

REMARKS/ARGUMENTS

Claims 1-36 are pending. Claims 1-31 have been rejected, but Applicants have presumed that Claims 1-36 were meant to be rejected in the Final Rejection dated September 8, 2004. New claim 37, which is dependent from Claim 1, has been added and is supported on page 8, lines 3-7. Claims 32 and 33 have been amended to cancel an inadvertent "t" present in these claims.

THE §112 REJECTION

Claims 1-31 have been rejected under 35 U.S.C §112, second paragraph, as being indefinite for failing to point out and distinctly claim the subject matter which applicants regard as the invention. Applicants respectfully disagree and respond as follows.

The Office Action gives two reasons as to why the claims are indefinite. The first reason as stated by the Office Action is:

"Where applicant acts has his own lexicographer to specifically define a term of a claim contrary to its ordinary meaning, the written description must clearly redefine the claim term . . . It appears that the 'box counting dimension' in the claims is used by the claim to mean 'packing density'. . . . The term is indefinite because the specification does not clearly redefine the term."

The second reason as stated by the Office is:

“It appears from the reading of the specification that this [box counting dimension] is based on a software product and entails parameters of pore size and number of spheres, that is a pore channel size. The use of a non-standard, such as a software program is viewed as indefinite, because these programs may change over time, . . .”

Applicants use the box counting dimension of the surface structure as it is known in the art. That is, the box counting dimension has not been used in any way contrary to its ordinary meaning. The “box counting dimension” or also commonly referred to as the “fractal dimension” as determined by the box counting method of a surface is a well known parameter in heterogeneous catalysis. This is shown by the more than 200 citations given by a search of the open literature, which is attached. Typically, in heterogeneous catalysis the fractal dimension is determined on a scale much less than 1 micrometer by employing adsorbed gas molecules of different sizes, which is illustrated in the enclosed articles, *Colloids and Surfaces, Physiochemical and Engineering Aspects*, 187-188 (2001) 257-265 and *Catalysis Letters*, 2(1989) 191-200. In addition, the box counting dimension or fractal dimension has been used and described in the patent art such as in U.S. Pat. Nos. 5,307,292; 5,444,795; 5,666,169; 5,719,784; 5,848,177; 5,982,386 and 6,143,158. The box counting method is specifically described as using one known in the fractal art “such as those described by Falconer, *Fractal Geometry Mathematical Foundations and Applications*, John Wiley and Sons, NY,” in which the pertinent section is enclosed. (page 6, lines 2-6 of the specification).

The only difference with the above cited heterogeneous catalysis art utilizing a fractal/box counting dimension is that, applicants have discovered a surprising result for the catalytic treatment of exhaust gas. The surprising result arises when the fractal/box counting dimension is at least 1.2 for a catalyst-substrate surface wherein the fractal/box counting dimension is determined on a scale greater than 1 micrometer to about 1 mm. The box counting methodology does not change from the above cited heterogeneous catalysis art above except that the boxes or spheres used to cover the surface when measuring the surface's box counting dimension must be larger than probe gas molecules. To do this, the commercially available software was merely cited in the specification to teach a convenient way of producing the boxes/spheres in applying the box counting method, for example, to the micrographs in the specification (page 6, lines 8-26).

To illustrate the box counting method, a surface is covered by spheres or boxes (squares) of varying sizes and the amount of spheres or boxes counted, where differing rules of placement of the boxes or spheres may be used as long as it is self consistent as illustrated in Falconer on page 40. The box counting/fractal dimension is then determined merely by plotting the log of the number of boxes versus the log of the size of the boxes wherein the slope of the line is the box counting/fractal dimension in the size range selected as described by the specification on page 6, lines 8-26 and described on page 37-40 of Falconer. The surface box counting method is depicted in the following illustrations 1-4.

Illustration 1; Idealized micrograph of a cross-section of a surface.

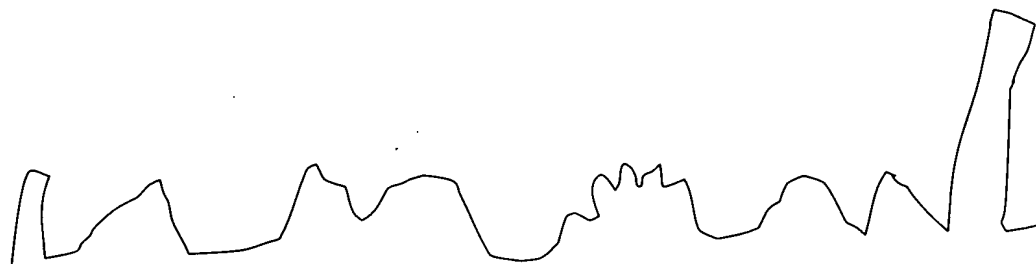


Illustration 2: Idealized surface covered with smaller spheres.

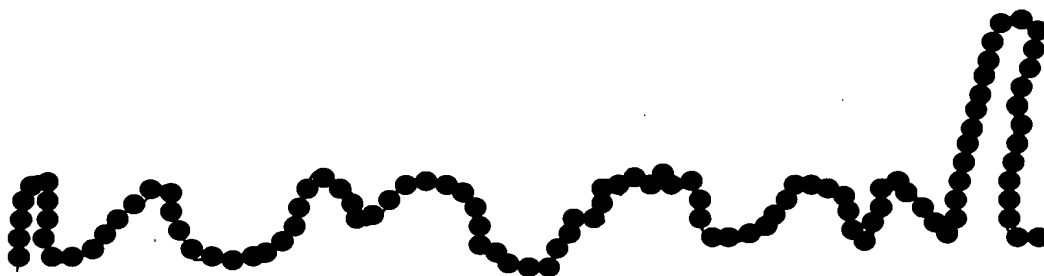


Illustration 3: Idealized surface covered with larger spheres.

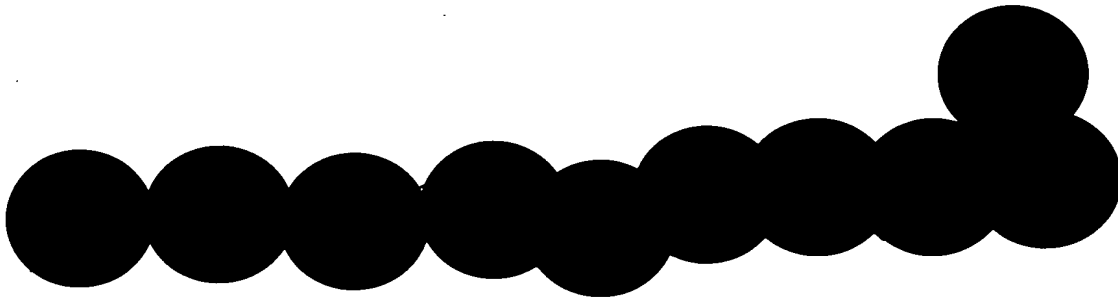
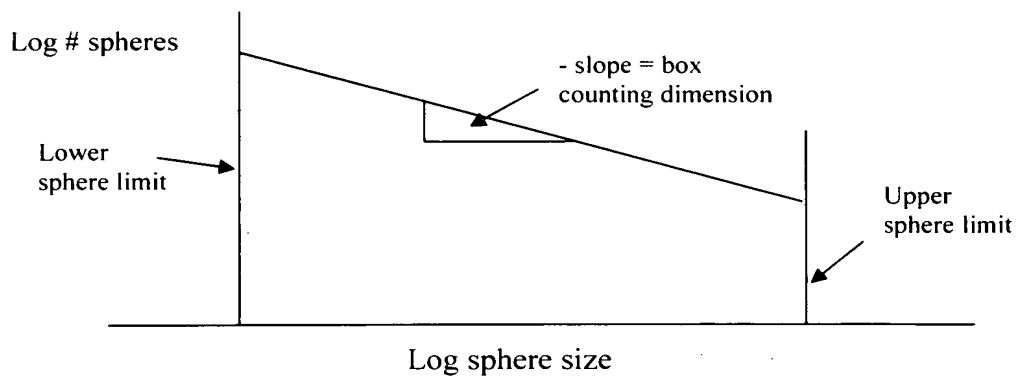


Illustration 4: Log-log plot of number of spheres v. sphere size



Since applicants specifically describe and use the box counting method to determine the fractal/box counting dimension consistent with its ordinary meaning and the software is merely cited in the specification as a convenient way of producing

the boxes when analyzing a micrograph of a cross-section of the catalyst-substrate surface, Independent Claims 1, 2 and 16 and Claims dependent therefrom are definite.

THE §102(b) REJECTION

Claims 1, 2 and 4-22 have been rejected under 35 U.S.C. §103(b) as being anticipated by Guile et al., U.S. Pat. No. 5,716,899 (Guile herein). Applicants respectfully disagree and respond as follows.

Applicants invention, in claims 1, 2 and 16, is a catalytic device that is comprised of a ceramic support of fused ceramic grains and a catalyst in which the surface is defined by a box counting dimension. The smallest box used to determine the box counting dimension is 1 micrometer. That is, any feature of the surface on the order of 1 micrometer or smaller is disregarded and as such will not impact the box counting dimension (i.e., will render a box counting dimension of 1 or close to 1). Claims 1, 2 and 16 make it clear that the surface is significantly fractal in nature or if periodic a bed of nails type structure where the surface feature is at least greater than 1 micrometer.

In contrast, Guile describes a bare (i.e., honeycomb without a catalyst) porous honeycomb that has pores having an average diameter of about 15 to 30 micrometers. (col. 4, lines 13-20). Guile, then, specifically describes that the pores of the bare honeycomb are filled with "active" material or in other words a catalyst. (col. 4, lines 40-45). Thus, the surface of Guile now is a surface that is either dense flat honeycomb surface or flat catalyst surface as shown in Fig. 2a. The activated carbon particles have pores on the order of 10 to 15 angstroms, which is much smaller than the lower limit of the box counting dimension. (col. 5, lines 50-56). The following

Figures 1 and 2 illustrate the bare substrate and an idealized filled “catalyzed” substrate of Guile.

Fig. 1: Bare substrate having pores.

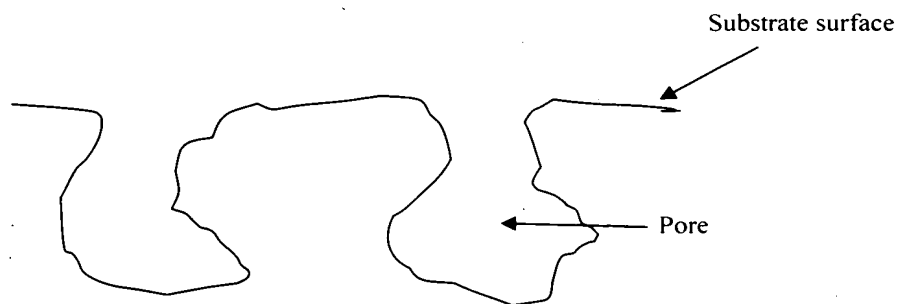
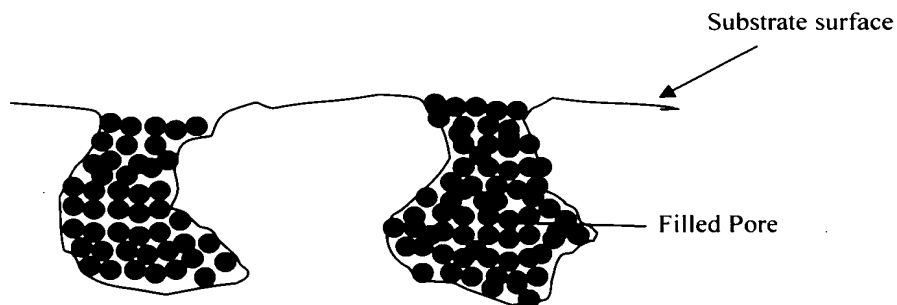


Fig. 2; Guile substrate where pores are filled with catalyst particles.



From Guile, the catalyst particles must be substantially smaller than the pores of the honeycomb body, otherwise they would not fill the pores. (col. 6, lines 12-14). The catalyst particles are ground and the median particle diameter after grinding is about 2-6 micrometers. It is well known that monospheres of particles closed packed will result in a pore diameter of less than 1 micrometer. (See page 190 of Introduction to the Principles of Ceramic Processing, James S. Reed, Wiley Interscience, New

York, NY, 1988, previously submitted). It is also well known that continuous size distributions of particles, such as those arising from ball milling as in Guile, will pack much more efficiently (the larger pores are filled by the smaller particles). *id.* The resulting Guile catalyst-substrate surface, by first principles, does not create the required surface of the present invention because the pores and features of the surface will not have features even remotely greater than 1 micrometer. That is Guile's catalyst-substrate surface will have pores less than 1 micrometer and as such a sphere or box having a dimension of 1 micrometer or larger will span such a pore and as such will appear as smooth surface (straight line) in the box counting method as exemplified in illustration 3 above. Because Guile's catalyst-substrate surface will appear as a straight line in the box counting method it will have a fractal/box counting dimension that is or is nearly 1. Consequently, Claims 1, 2 and 4-22 are novel.

In addition, since Guile specifically creates a surface that fills in all of the pores with fine particles, Guile teaches away from the surface structure of Applicants invention. For this reason, Independent Claims 1, 2 and 16 and Claims dependent therefrom are non-obvious over Guile.

THE §103(a) REJECTION

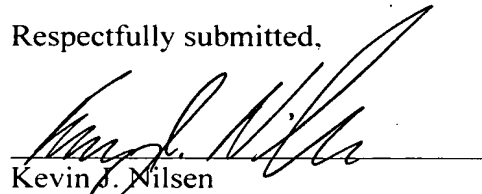
Claim 3 has been rejected under 35 U.S.C. §103(a) as being unpatentable over Guile, as stated in the above paragraph (referring to the Office Action's 102(b) rejection), and further in view of Moyer et al., U.S. Pat. No. 5,194,154 (Moyer herein). Claims 23-31 have been rejected as being unpatentable over Guile in view of Fukui et al., U.S. Pat. No. 5,569,455.

As stated above, Guile specifically teaches to fill in the pores with fine catalyst particles, which is opposite of the surface as required in independent Claim 1, 2 and

16. Even if Guile was combined with Moyer, the mullite honeycomb would be filled with catalyst particles such that the same structure of Guile would result. That is Guile would fill all the pores between the mullite grains making a surface not having features (pores) greater than 1 micrometer and as such would not create the present invention. Consequently, Guile in view of Moyer fails to teach the invention, but teaches away from the invention of Claims 1, 2 and 16. For this reason Claims 1, 2, and 16 and Claims dependent therefrom are non-obvious over Guile in view of Moyer.

Considering the foregoing reasons, Independent Claims 1, 2 and 16 and Claims dependent therefrom are patentable. Applicants, therefore, respectfully request withdrawal of all rejections and allowance of Claims 1-37.

Respectfully submitted,



Kevin J. Nilsen
Registration No. 41,510
Phone: 989-638-6505

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P. O. Box 1967
Midland, MI 48641-1967
KJN/caa

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FRACTAL GEOMETRY

Mathematical Foundations
and Applications

Kenneth Falconer

Reader in Mathematics, University of Bristol

JOHN WILEY & SONS

Chapter 3 Alternative definitions of dimension

Hausdorff dimension, discussed in the last chapter, is the principal definition of dimension that we shall work with. However, other definitions are in widespread use, and it is appropriate to examine some of these and their inter-relationship. Not all definitions are generally applicable—some only describe particular classes of set, such as curves.

Fundamental to most definitions of dimension is the idea of 'measurement at scale δ '. For each δ , we measure a set in a way that ignores irregularities of size less than δ , and we see how these measurements behave as $\delta \rightarrow 0$. For example, if F is a plane curve, then our measurement, $M_\delta(F)$, might be the number of steps required by a pair of dividers set at length δ to traverse F . A dimension of F is then determined by the power law (if any) obeyed by $M_\delta(F)$ as $\delta \rightarrow 0$. If

$$M_\delta(F) \sim c\delta^{-s} \quad (3.1)$$

for constants c and s , we might say that F has 'dimension' s , with c regarded as the ' s -dimensional length' of F . Taking logarithms

$$\log M_\delta(F) \simeq \log c - s \log \delta \quad (3.2)$$

in the sense that the difference of the two sides tends to 0 with δ , and

$$s = \lim_{\delta \rightarrow 0} \frac{\log M_\delta(F)}{-\log \delta}. \quad (3.3)$$

These formulae are appealing for computational or experimental purposes, since s can be estimated as the gradient of a log-log graph plotted over a suitable range of δ ; see figure 3.1. (Of course, for real phenomena, we can only work with a finite range of δ ; theory and experiment diverge before an atomic scale is reached; see Chapter 18.)

There may be no exact power law for $M_\delta(F)$, and the closest we can get to (3.3) are the lower and upper limits.

For the value of s given by (3.1) to behave like a dimension, the method of measurement needs to scale with the set, so that doubling the size of F and at the same time doubling the scale at which measurement takes place does not affect the answer; that is, we require $M_\delta(\delta F) = M_1(F)$ for all δ . If we modify our example and redefine $M_\delta(F)$ to be the sum of the divider step lengths then $M_\delta(F)$

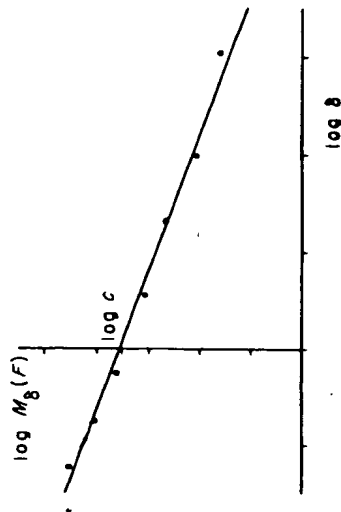


Fig 3

Figure 3.1 Empirical estimation of a dimension of a set F , on the power-law assumption $M_\delta(F) \sim c\delta^{-s}$.

is homogeneous of degree 1, i.e. $M_\delta(\delta F) = \delta^1 M_1(F)$ for $\delta > 0$, and this must be taken into account when defining the dimension. In general, if $M_\delta(F)$ is homogeneous of degree d , that is $M_\delta(\delta F) = \delta^d M_1(F)$, then a power law of the form $M_\delta(F) \sim c\delta^{d-s}$ corresponds to a dimension s .

There are no hard and fast rules for deciding whether a quantity may reasonably be regarded as a dimension. There are many definitions that do not fit exactly into the above, rather simplified, scenario. The factors that determine the acceptability of a definition of a dimension are recognized largely by experience and intuition. In general one looks for some sort of scaling behaviour, a naturalness of the definition in the particular context and properties typical of dimensions such as those discussed below.

A word of warning: as we shall see, apparently similar definitions of dimension can have widely differing properties. It should not be assumed that different definitions give the same value of dimension, even for 'nice' sets. Such assumptions have led to major misconceptions and confusion in the past. It is necessary to derive the properties of any 'dimension' from its definition. The properties of Hausdorff dimension (on which we shall largely concentrate in the later chapters of this book) do not necessarily all hold for other definitions.

What are the desirable properties of a 'dimension'? Those derived in the last chapter for Hausdorff dimension are fairly typical.

Monotonicity. If $E \subset F$ then $\dim_H E \leq \dim_H F$.

Stability. $\dim_H(E \cup F) = \max(\dim_H E, \dim_H F)$.

Countable stability. $\dim_H(\bigcup_{i=1}^{\infty} F_i) = \sup_{i \leq i < \infty} \dim_H F_i$.

Geometric invariance. $\dim_H f(F) = \dim_H F$ if f is a transformation of \mathbb{R}^n such as a translation, rotation, similarity or affinity.

Lipschitz invariance. $\dim_H f(F) = \dim_H F$ if f is a bi-Lipschitz transformation.

Countable sets. $\dim_H F = 0$ if F is finite or countable.

Open sets. If F is an open subset of \mathbb{R}^n then $\dim_H F = n$.

Smooth manifolds. $\dim_H F = m$ if F is a smooth m -dimensional manifold.

All definitions of dimension are monotonic, most are stable, but, as we shall see, some common definitions fail to exhibit countable stability and may have

countable sets of positive dimension. All the usual dimensions are Lipschitz invariant, and, therefore, geometrically invariant. The 'open sets' and 'smooth manifolds' properties ensure that the dimension is an extension of the classical definition. Note that different definitions of dimension can provide different information about which sets are Lipschitz equivalent.

3.1 Box-counting dimensions

Box-counting or box dimension is one of the most widely used dimensions. Its popularity is largely due to its relative ease of mathematical calculation and empirical estimation. The definition goes back at least to the 1930s and it has been variously termed Kolmogorov entropy, entropy dimension, capacity dimension (a term best avoided in view of potential theoretic associations), metric dimension, logarithmic density and information dimension. We shall always refer to box or box counting dimension to avoid confusion.

Let F be any non-empty bounded subset of \mathbb{R}^n and let $N_\delta(F)$ be the smallest number of sets of diameter at most δ which can cover F . The lower and upper box-counting dimensions of F respectively are defined as

$$\underline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \quad (3.4)$$

$$\overline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta}. \quad (3.5)$$

If these are equal we refer to the common value as the box-counting dimension or box dimension of F

$$\dim_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta}. \quad (3.6)$$

There are several equivalent definitions of box dimension that are sometimes more convenient to use. Consider the collection of cubes in the δ -coordinate mesh of \mathbb{R}^n , i.e. cubes of the form

$$[m_1\delta, (m_1 + 1)\delta] \times \cdots \times [m_n\delta, (m_n + 1)\delta]$$

where m_1, \dots, m_n are integers. (Recall that a 'cube' is an interval in \mathbb{R}^1 and a square in \mathbb{R}^2 .) Let $N'_\delta(F)$ be the number of δ -mesh cubes that intersect F . They obviously provide a collection of $N'_\delta(F)$ sets of diameter $\delta\sqrt{n}$ that cover F , so

$$N_{\delta\sqrt{n}}(F) \leq N'_\delta(F).$$

If $\delta\sqrt{n} < 1$ then

$$\frac{\log N_{\delta\sqrt{n}}(F)}{-\log(\delta\sqrt{n})} \leq \frac{\log N'_\delta(F)}{-\log \sqrt{n} - \log \delta}$$

so taking limits as $\delta \rightarrow 0$

$$\underline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N'_\delta(F)}{-\log \delta} \quad (3.7)$$

and

$$\overline{\dim}_B F \leq \lim_{\delta \rightarrow 0} \frac{\log N'_\delta(F)}{-\log \delta}. \quad (3.8)$$

On the other hand, any set of diameter at most δ is contained in 3^n mesh cubes of side δ (by choosing a cube containing some point of the set together with its neighbouring cubes). Thus

$$N'_\delta(F) \leq 3^n N_\delta(F)$$

and taking logarithms leads to the opposite inequalities to (3.7) and (3.8). Hence to find the box dimensions (3.4)–(3.6), we can equally well take $N_\delta(F)$ to be the number of mesh cubes of side δ that intersect F .

This version of the definitions is widely used empirically. To find the box dimension of a plane set F we may draw a mesh of squares or boxes of side δ and count the number $N_\delta(F)$ that overlap the set for various small δ (hence the name 'box counting'). The dimension is the logarithmic rate at which $N_\delta(F)$ increases as $\delta \rightarrow 0$, and may be estimated by the gradient of the graph of $\log N_\delta(F)$ against $-\log \delta$.

This definition gives an interpretation of the meaning of box dimension. The number of mesh cubes of side δ that intersect a set is an indication of how spread out or irregular the set is when examined at scale δ . The dimension reflects how rapidly the irregularities develop as $\delta \rightarrow 0$.

Another frequently used definition of box dimension is obtained by taking $N_\delta(F)$ in (3.4)–(3.6) to be the smallest number of arbitrary cubes of side δ required to cover F . The equivalence of this definition follows as in the mesh cube case, noting that any cube of side δ has diameter $\delta\sqrt{n}$, and that any set of diameter of at most δ is contained in a cube of side δ .

Similarly, we get exactly the same values if in (3.4)–(3.6) we take $N_\delta(F)$ as the smallest number of closed balls of radius δ that cover F .

A less obviously equivalent formulation of box dimension involves the largest number of disjoint balls of radius δ with centres in F . Let this number be $N'_\delta(F)$, and let $B_1, \dots, B_{N'_\delta(F)}$ be disjoint balls centred in F and of radius δ . If x belongs to F then x must be within distance δ of one of the B_i , otherwise the ball of centre x and radius δ can be added to form a larger collection of disjoint balls. Thus the $N'_\delta(F)$ balls concentric with the B_i but of radius 2δ (diameter 4δ) cover F , giving

$$N_{4\delta}(F) \leq N'_\delta(F). \quad (3.9)$$

On the other hand, suppose that $B_1, \dots, B_{N'_\delta(F)}$ are disjoint balls of radii δ with centres in F . Let U_1, \dots, U_k be any collection of sets of diameter at most δ which cover F . Since the U_i must cover the centres of the B_i , each B_i must

contain at least one of the U_j . As the B_i are disjoint there are at least as many U_j as B_i . Hence

$$N'_\delta(F) \leq N_\delta(F). \quad (3.10)$$

Taking logarithms of (3.9) and (3.10) shows that the values of (3.4)–(3.6) are unaltered if $N_\delta(F)$ is replaced by this $N'_\delta(F)$.

These various definitions are summarized below and in figure 3.2.

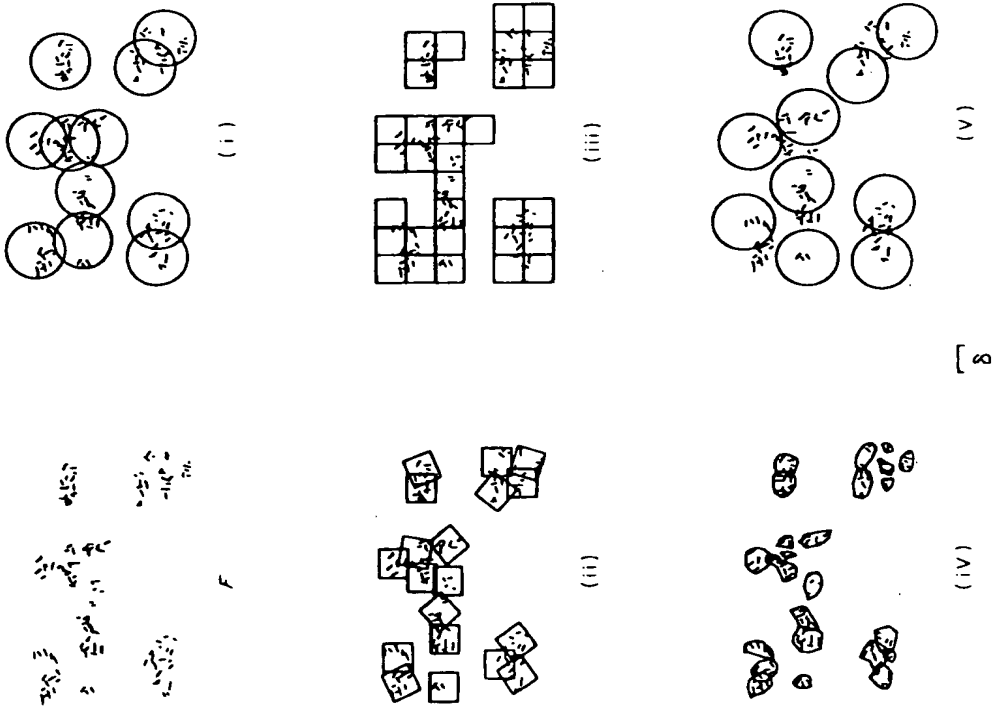


Figure 3.2 Five ways of finding the box dimension of F ; see Equivalent definitions 3.1. The number $N_\delta(F)$ is taken to be: (i) the least number of closed balls of radius δ that cover F ; (ii) the least number of cubes of side δ that cover F ; (iii) the number of δ -mesh cubes that intersect F ; (iv) the least number of sets of diameter at most δ that cover F ; (v) the greatest number of disjoint balls of radius δ with centres in F .

Equivalent definitions 3.1

The lower and upper box-counting dimensions of a subset F of \mathbb{R}^n are given by

$$\underline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \quad (3.11)$$

$$\overline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \quad (3.12)$$

and the box-counting dimension of F by

$$\dim_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \quad (3.13)$$

(if this limit exists), where $N_\delta(F)$ is any of the following:

- (i) the smallest number of closed balls of radius δ that cover F ;
- (ii) the smallest number of cubes of side δ that cover F ;
- (iii) the number of δ -mesh cubes that intersect F ;
- (iv) the smallest number of sets of diameter at most δ that cover F ;
- (v) the largest number of disjoint balls of radius δ with centres in F .

This list could be extended further; in practice one adopts the definition most convenient for a particular application.

It is worth noting that, in (3.11)–(3.13), it is enough to consider limits as δ tends to 0 through any decreasing sequence δ_k such that $\delta_{k+1} \geq c\delta_k$ for some constant $0 < c < 1$; in particular for $\delta_k = c^k$. To see this, note that if $\delta_{k+1} \leq \delta < \delta_k$, then

$$\frac{\log N_\delta(F)}{-\log \delta} \leq \frac{\log N_{\delta_{k+1}}(F)}{-\log \delta_k} \leq \frac{\log N_{\delta_{k+1}}(F)}{-\log \delta_{k+1} + \log(\delta_{k+1}/\delta_k)} \leq \frac{\log N_{\delta_{k+1}}(F)}{-\log \delta_{k+1} + \log c}$$

and so

$$\lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \leq \lim_{k \rightarrow \infty} \frac{\log N_{\delta_k}(F)}{-\log \delta_k}. \quad (3.14)$$

The opposite inequality is trivial; the case of lower limits may be dealt with in the same way.

There is an equivalent definition of box dimension of a rather different form that is worth mentioning. Recall that the δ -parallel body F_δ of F is

$$F_\delta = \{x \in \mathbb{R}^n : |x - y| \leq \delta \text{ for some } y \in F\} \quad (3.15)$$

i.e. the set of points within distance δ of F . We consider the rate at which the n -dimensional volume of F_δ shrinks as $\delta \rightarrow 0$. In \mathbb{R}^3 , if F is a single point then F_δ is a ball with $\text{vol}(F_\delta) = \frac{4}{3}\pi\delta^3$, if F is a segment of length l then F_δ is 'sausage-like' with $\text{vol}(F_\delta) \sim \pi l\delta^2$, and if F is a flat set of area a then F_δ is essentially a thickening of F with $\text{vol}(F_\delta) \sim 2a\delta$. In each case, $\text{vol}(F_\delta) \sim c\delta^{3-s}$ where the integer s is the dimension of F , so that exponent of δ is indicative of the

dimension. The coefficient c of δ^{3-s} , known as the *Minkowski content* of F , is a measure of the length, area or volume of the set as appropriate.

This idea extends to fractional dimensions. If F is a subset of \mathbb{R}^n and, for some s , $\text{vol}^n(F_\delta)/\delta^{n-s}$ tends to a positive finite limit as $\delta \rightarrow 0$, then it makes sense to regard F as s -dimensional. The limiting value is called the s -dimensional *content* of F —a concept of slightly restricted use since it is not necessarily additive on disjoint subsets, i.e. is not a measure. Even if this limit does not exist, we may be able to extract the critical exponent of δ and this turns out to be related to the box dimension.

Proposition 3.2

If F is a subset of \mathbb{R}^n , then

$$\begin{aligned}\underline{\dim}_B F &= n - \lim_{\delta \rightarrow 0} \frac{\log \text{vol}^n(F_\delta)}{\log \delta} \\ \overline{\dim}_B F &= n - \lim_{\delta \rightarrow 0} \frac{\log \text{vol}^n(F_\delta)}{\log \delta}\end{aligned}$$

where F_δ is the δ -parallel body to F .

Proof. If F can be covered by $N_\delta(F)$ balls of radius δ then F_δ can be covered by the concentric balls of radius 2δ . Hence

$$\text{vol}^n(F_\delta) \leq N_\delta(F) c_n (2\delta)^n$$

where c_n is the volume of the unit ball in \mathbb{R}^n . Taking logarithms,

$$\frac{\log \text{vol}^n(F_\delta)}{-\log \delta} \leq \frac{\log 2^n c_n + n \log \delta + \log N_\delta(F)}{-\log \delta}$$

gives

$$\lim_{\delta \rightarrow 0} \frac{\log \text{vol}^n(F_\delta)}{-\log \delta} \leq -n + \underline{\dim}_B F \quad (3.16)$$

with a similar inequality for the upper limits. On the other hand if there are $N_\delta(F)$ disjoint balls of radius δ with centres in F , then

$$N_\delta(F) c_n (2\delta)^n \leq \text{vol}^n(F_\delta).$$

Taking logarithms gives the opposite inequality to (3.16), using Equivalent definition 3.1(v). \square

Because of Proposition 3.2, box dimension is sometimes referred to as *Minkowski dimension*.

It is important to understand the relationship between box-counting dimension and Hausdorff dimension. If F can be covered by $N_\delta(F)$ sets of diameter δ , then, from definition (2.1),

$$\mathcal{H}_\delta^s(F) \leq N_\delta(F) \delta^s.$$

If $1 < \mathcal{H}^s(F) = \lim_{\delta \rightarrow 0} \mathcal{H}_\delta^s(F)$ then $\log N_\delta(F) + s \log \delta > 0$ if δ is sufficiently small. Thus $s \leq \underline{\lim}_{\delta \rightarrow 0} \log N_\delta(F) / -\log \delta$ so

$$\underline{\dim}_B F \leq \underline{\lim}_{\delta \rightarrow 0} F \leq \underline{\dim}_B F \quad (3.17)$$

for any $F \subset \mathbb{R}^n$. We do *not* in general get equality here. Although Hausdorff and box dimensions are equal for many 'reasonably regular' sets, there are plenty of examples where this inequality is strict.

Roughly speaking (3.6) says that $N_\delta(F) \approx \delta^{-s}$ for small δ , where $s = \underline{\dim}_B F$. More precisely, it says that

$$N_\delta(F) \delta^s \rightarrow \infty \quad \text{if } s < \underline{\dim}_B F$$

and

$$N_\delta(F) \delta^s \rightarrow 0 \quad \text{if } s > \underline{\dim}_B F.$$

But

$$N_\delta(F) \delta^s = \inf \left\{ \sum_i \delta^{s_i} : \{U_i\} \text{ is a (finite) } \delta\text{-cover of } F \right\},$$

which should be compared with

$$\mathcal{H}_\delta^s(F) = \inf \left\{ \sum_i |U_i|^s : \{U_i\} \text{ is a } \delta\text{-cover of } F \right\},$$

which occurs in the definition of Hausdorff measure and dimension. In calculating Hausdorff dimension, we assign different weights $|U_i|^s$ to the covering sets U_i , whereas for the box dimensions we use the same weight δ^s for each covering set. Box dimensions may be thought of as indicating the efficiency with which a set may be covered by small sets of equal size, whereas Hausdorff dimension involves coverings by sets of small but perhaps widely varying size.

There is a temptation to introduce the quantity $v(F) = \lim_{\delta \rightarrow 0} N_\delta(F) \delta^s$, but this does *not* give a measure on subsets of \mathbb{R}^n . As we shall see, one consequence of this is that box dimensions have a number of unfortunate properties, and can be awkward to handle mathematically.

Since box dimensions are determined by coverings by sets of equal size they tend to be easier to calculate than Hausdorff dimensions.

Example 3.3

Let F be the middle third Cantor set. Then $\underline{\dim}_B F = \underline{\dim}_B F = \log 2 / \log 3$.

Calculation. The obvious covering by the 2^k intervals of E_k of length 3^{-k} gives that $N_\delta(F) \leq 2^k$ if $3^{-k} < \delta \leq 3^{-k+1}$. From (3.5)

$$\underline{\dim}_B F = \lim_{\delta \rightarrow 0} \frac{\log N_\delta(F)}{-\log \delta} \leq \lim_{k \rightarrow \infty} \frac{\log 2^k}{\log 3^{k-1}} = \frac{\log 2}{\log 3}.$$

On the other hand, any interval of length δ with $3^{-k-1} \leq \delta < 3^{-k}$ intersects at

most one of the basic intervals of length 3^{-k} used in the construction of F . There are 2^k such intervals so at least 2^k intervals of length δ are required to cover F . Hence $N_\delta(F) \geq 2^k$ leading to $\dim_B F \geq \log 2 / \log 3$. \square

Thus, at least for the Cantor set, $\dim_H F = \dim_B F$.

3.2 Properties and problems of box-counting dimension

The following elementary properties of box dimension mirror those of Hausdorff dimension, and may be verified in much the same way.

- (i) A smooth m -dimensional submanifold of \mathbb{R}^n has $\dim_B F = m$.
- (ii) \dim_B and $\overline{\dim}_B$ are monotonic.
- (iii) $\overline{\dim}_B$ is finitely stable, i.e.

$$\overline{\dim}_B(E \cup F) = \max\{\overline{\dim}_B E, \overline{\dim}_B F\}$$

though \dim_B is not.

- (iv) \dim_B and $\overline{\dim}_B$ are Lipschitz invariant. This is so because, if $|f(x) - f(y)| \leq c|x - y|$ and F can be covered by $N_\delta(F)$ sets of diameter at most δ , then the $N_\delta(F)$ images of these sets under f form a cover by sets of diameter at most $c\delta$, thus $\dim_B f(F) \leq \dim_B F$. Similarly, box dimensions behave just like Hausdorff dimensions under bi-Lipschitz and Hölder transformations.

We now start to encounter the disadvantages of box-counting dimension. The next proposition is at first appealing, but has undesirable consequences.

Proposition 3.4

Let \bar{F} denote the closure of F (i.e. the smallest closed subset of \mathbb{R}^n containing F). Then

$$\dim_B \bar{F} = \dim_B F$$

and

$$\overline{\dim}_B \bar{F} = \overline{\dim}_B F.$$

Proof. Let B_1, \dots, B_k be a finite collection of closed balls of radii δ . If the closed set $\bigcup_{i=1}^k B_i$ contains F , it also contains \bar{F} . Hence the smallest number of closed balls of radius δ that cover F is enough to cover the larger set \bar{F} . The result follows. \square

An immediate consequence of this is that if F is a dense subset of an open region of \mathbb{R}^n then $\dim_B F = \overline{\dim}_B F = n$. For example, let F be the (countable) set of rational numbers between 0 and 1. Then \bar{F} is the entire interval $[0, 1]$.

so that $\dim_B F = \overline{\dim}_B F = 1$. Thus countable sets can have non-zero box dimension. Moreover, the box-counting dimension of each rational number regarded as a one-point set is clearly zero, but the countable union of these singleton sets has dimension 1. Consequently, it is not generally true that $\dim_B \bigcup_{i=1}^\infty F_i = \sup_i \dim_B F_i$.

This severely limits the usefulness of box dimension—introducing a small, i.e. countable, set of points can play havoc with the dimension. We might hope to salvage something by restricting attention to closed sets, but difficulties still remain.

Example 3.5

$F = \{0, 1, \frac{1}{2}, \frac{1}{3}, \dots\}$ is a compact set with $\dim_B F = \frac{1}{2}$.

Calculation. If $|U| = \delta < \frac{1}{2}$ and k is the integer satisfying $1/(k-1)k > \delta \geq 1/k(k+1)$ then U can cover at most one of the points $\{1, \frac{1}{2}, \dots, 1/k\}$. Thus at least k sets of diameter δ are required to cover F , so

$$\frac{\log N_\delta(F)}{-\log \delta} \geq \frac{\log k}{\log k(k+1)}.$$

Letting $\delta \rightarrow 0$ gives $\dim_B F \geq \frac{1}{2}$. On the other hand, if $\frac{1}{2} > \delta > 0$, take k such that $1/(k-1)k > \delta \geq 1/k(k+1)$. Then $(k+1)$ intervals of length δ cover $[0, 1/k]$, leaving $k-1$ points of F which can be covered by another $k-1$ intervals. Thus

$$\frac{\log N_\delta(F)}{-\log \delta} \leq \frac{\log(2k)}{\log k(k-1)}$$

giving

$$\overline{\dim}_B F \leq \frac{1}{2}.$$

\square

No-one would regard this set, with all but one of its points isolated, as a fractal, yet it has fractional box dimension.

Nevertheless, as well as being convenient in practice, box dimensions are very useful in theory. If, as often happens, it can be shown that a set has equal box and Hausdorff dimensions, the interplay of these definitions can be used to powerful effect.

3.3 Modified box-counting dimensions

There are ways of overcoming the difficulties of box dimension outlined in the last section. However, they will probably not appeal to the user since they re-introduce all the difficulties of calculation associated with Hausdorff dimension and more.

If F is a subset of \mathbb{R}^n we can try to decompose F into a countable number of pieces F_1, F_2, \dots in such a way that the largest piece has as small a dimension as possible. This idea leads to the following *modified box-counting dimensions*:

$$\underline{\dim}_{\text{MB}} F = \inf \left\{ \sup_i \underline{\dim}_{\text{MB}} F_i : F \subset \bigcup_{i=1}^{\infty} F_i \right\} \quad (3.18)$$

$$\overline{\dim}_{\text{MB}} F = \inf \left\{ \sup_i \overline{\dim}_{\text{MB}} F_i : F \subset \bigcup_{i=1}^{\infty} F_i \right\}. \quad (3.19)$$

(In both cases the infimum is over all possible countable covers $\{F_i\}$ of F .) Clearly $\underline{\dim}_{\text{MB}} F \leq \underline{\dim}' F$ and $\overline{\dim}_{\text{MB}} F \leq \overline{\dim}_{\text{MB}} F$. However, we now have that $\underline{\dim}_{\text{MB}} F = \underline{\dim}' F = 0$ if F is countable—just take the F_i to be one-point sets. Moreover, for any subset F of \mathbb{R}^n ,

$$0 \leq \underline{\dim}_{\text{H}} F \leq \underline{\dim}_{\text{MB}} F \leq \overline{\dim}_{\text{MB}} F \leq \overline{\dim}_{\text{B}} F \leq n. \quad (3.20)$$

It is easy to see that $\underline{\dim}_{\text{MB}}$ and $\overline{\dim}_{\text{MB}}$ recover all the desirable properties of a dimension, but they can be hard to calculate. However, there is a useful test for compact sets to have equal box and modified box dimensions. It applies to sets that might be described as 'dimensionally homogeneous'.

Proposition 3.6

Let $F \subset \mathbb{R}^n$ be compact. Suppose that

$$\overline{\dim}_{\text{B}}(F \cap V) = \overline{\dim}_{\text{B}} F \quad (3.21)$$

for all open sets V that intersect F . Then $\overline{\dim}_{\text{B}} F = \overline{\dim}_{\text{MB}} F$. A similar result holds for lower box-counting dimensions.

Proof. Let $F \subset \bigcup_{i=1}^{\infty} F_i$ with each F_i closed. A version of Baire's category theorem (which may be found in any text on basic general topology, and which we quote without proof) states that there is an index i and an open set $V \subset \mathbb{R}^n$ such that $F \cap V \subset F_i$. For this i , $\overline{\dim}_{\text{B}} F_i = \overline{\dim}_{\text{B}} F$. Using (3.19) and Proposition 3.4

$$\begin{aligned} \overline{\dim}_{\text{MB}} F &= \inf \left\{ \sup_i \overline{\dim}_{\text{B}} F_i : F \subset \bigcup_{i=1}^{\infty} F_i \text{ where the } F_i \text{ are closed sets} \right\} \\ &\geq \overline{\dim}_{\text{B}} F. \end{aligned}$$

The opposite inequality is contained in (3.20). A similar argument deals with the lower dimensions. \square

For an application suppose that F is a compact set with a high degree of self-similarity, for instance the middle third Cantor set or von Koch curve. If V is any open set that intersects F , then $F \cap V$ contains a geometrically similar

copy of F which must have upper box dimension equal to that of F , so that (3.21) holds.

•3.4 Packing measures and dimensions

Unlike Hausdorff dimension, neither the box dimensions or modified box dimensions are defined in terms of measures, and this can present difficulties in their theoretical development. Nevertheless, the circle of ideas in the last section may be completed in a way that is, at least mathematically, elegant. Recall that Hausdorff dimension may be defined using economical coverings by small balls (2.16) whilst $\underline{\dim}_{\text{B}}$ may be defined using economical coverings by small balls of equal radius (Equivalent definition 3.1(i)). On the other hand $\underline{\dim}_{\text{B}}$ may be thought of as a dimension that depends on packings by disjoint balls of equal radius that are as dense as possible (Equivalent definition 3.1(v)). It is therefore natural to try to look for a dimension that is defined in terms of dense packings by disjoint balls of differing small radii.

We try to follow the pattern of definition of Hausdorff measure and dimension. Let

$$\begin{aligned} \mathcal{P}_{\delta}^*(F) &= \sup \left\{ \sum_i |B_i|^\delta : \{B_i\} \text{ is a collection of disjoint balls of radii } r_i \text{ at} \right. \\ &\quad \left. \text{most } \delta \text{ with centres in } F \right\}. \end{aligned} \quad (3.22)$$

Since $\mathcal{P}_{\delta}^*(F)$ decreases with δ , the limit

$$\mathcal{P}_0^*(F) = \lim_{\delta \rightarrow 0} \mathcal{P}_{\delta}^*(F) \quad (3.23)$$

exists. At this point we meet the problems encountered with box-counting dimensions. By considering countable dense sets it is easy to see that $\mathcal{P}_0^*(F)$ is not a measure. Hence we modify the definition to

$$\mathcal{P}^s(F) = \inf \left\{ \sum_i \mathcal{P}_0^s(F_i) : F \subset \bigcup_{i=1}^{\infty} F_i \right\}. \quad (3.24)$$

It may be shown that $\mathcal{P}^s(F)$ is a measure on \mathbb{R}^n , known as the *s-dimensional packing measure*. We may define the *packing dimension* in the usual way:

$$\dim_{\text{P}} F = \sup \{ s : \mathcal{P}^s(F) = \infty \} = \inf \{ s : \mathcal{P}^s(F) = 0 \}. \quad (3.25)$$

The underlying measure structure immediately implies that for a countable collection of sets $\{F_i\}$

$$\dim_{\text{P}} \left(\bigcup_{i=1}^{\infty} F_i \right) = \sup_i \dim_{\text{P}} F_i \quad (3.26)$$

since if $s > \dim_{\text{H}} F_i$ for all i , then $\mathcal{P}^s(\bigcup_i F_i) \leq \sum_i \mathcal{P}^s(F_i) = 0$, and $\dim_{\text{P}}(\bigcup_i F_i) \leq s$.

APPLICATIONS OF FRACTAL GEOMETRY FOR CHARACTERIZING HYDROTREATING CATALYSTS

C. FAIRBRIDGE

Energy Research Laboratories, Energy, Mines and Resources Canada, CANMET, 555 Booth Street, Ottawa, Ontario, Canada K1A 0G1

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The characterization of heterogeneous catalysts or porous solids involves a description of a reacting interface. The physical and chemical properties of catalysts – surface area, active site density and reactivity – have recently been quantified by fractal geometry. The use of fractal dimension rather than N_2 BET surface area provides for the determination of effective surface area for any adsorbate. The concept may be useful in predicting the reactivity of individual components in hydroprocessing. Similarly, the effects of particle size on surface area and reactivity, or the distribution of active sites on a catalyst, may be quantified by fractal geometry. Applications are discussed with specific examples.

1. Introduction

The geometry of a reacting interface is extremely important in most industrial reaction systems. In heterogeneous catalysis, the performance of a catalytic system is dictated by the geometry of the interface as well as by the chemical reactions which occur at that interface. The application of fractal geometry for characterizing boundaries or porous materials is currently receiving considerable attention. This paper discusses potential application of fractal geometry in heterogeneous catalysis, particularly hydroprocessing.

The concept of spatial dimension has normally been represented by integers. In classical Euclidean geometry, a line, rectangle or cube are described as one, two, or three-dimensional. The physical world, however, involves nontrivial geometries. Mandelbrot [1] introduced the term fractal as a dimensionless number which quantifies the degree of irregularity or ruggedness of a boundary. A fractal therefore is an object that has a fractional dimension. A rough surface, for example, may have an intermediate dimension between a 2-dimensional smooth surface and a 3-dimensional volume. The fractal dimension of a surface, D , is therefore a quantitative measure of the space-filling ability of that surface.

In the field of heterogeneous catalysis, the coupling of geometry and chemistry introduces the phenomenon of structure sensitivity. The complex geometry of the interface may be described quantitatively by a fractal dimension if the interface is

symmetric to transformations of scale, i.e., self-similar. This simply means that for a fractal, the same type of features are observed at different magnifications. In heterogeneous catalysis this change of scale can involve reactants of different molecular sizes (as in the sorption of a series of adsorbates), or catalyst particles of different sizes with the same reactants, or supported catalysts with varying amounts of active sites. Avnir and colleagues [2,3] have introduced two simple equations to quantify the scaling phenomena of surfaces. If a catalyst surface is a fractal, the accessible surface area, A , is related to catalyst particle radius, R , by:

$$A = k_1 R^{D-3} \quad (1)$$

where D is the surface fractal dimension. In addition, accessible surface area is related to the effective cross-sectional area of the adsorbate, a_m , by:

$$A = k_2 a_m^{(2-D)/2} \quad (2)$$

The surface fractal dimension is a very useful quantitative parameter for characterizing typical hydroprocessing catalysts.

Nitrogen BET specific surface area is most often used as a quantitative measure of surface area. The porous materials used as supports for hydrotreating catalysts – amorphous alumina and silica-alumina – have a surface fractal dimension between 2 and 3. The larger the fractal dimension, approaching 3, the more rugged the catalyst surface. In the limit, the surface will fill a volume of space. The concept of the space-filling ability of a catalyst leads to a slightly different approach in describing catalytic reactions. In effect, a catalytic reaction may not so much occur on a surface as in a surface. The active sites are normally viewed as elements of disorder – kinks, vacancies – when perhaps an alternate picture for hydroprocessing catalysts is an element of order in a disordered surface.

2. Discussion

The equations above are useful not only in measuring D but also in calculating accessible surface area, effective cross-sectional area of adsorbates or even particle size. For reactions of large molecules, the use of accessible surface area for each reactant/product is preferable to the use of N_2 BET surface area. Table 1 was calculated from eq. (2) for three hypothetical hydrotreating catalysts of surface fractal dimension $D = 2.10, 2.50$ or 2.90 . The proportionality constant was determined by assuming a value of $200 \text{ m}^2 \text{ g}^{-1}$ for the N_2 BET area, and then the accessible areas for benzene, naphthalene, and anthracene were calculated.

Similarly, by assuming an anthracene surface area of $100 \text{ m}^2 \text{ g}^{-1}$ the N_2 BET specific surface area can be calculated as in table 2.

The area occupied by an adsorbate molecule in a monolayer, a_m , was calculated from liquid density values [4]. The tables indicate that N_2 BET surface area

Table 1
Accessible surface area

adsorbate	a_m (nm ²)	Calculated accessible surface area (m ² g ⁻¹)		
		$D = 2.10$	$D = 2.50$	$D = 2.90$
nitrogen	0.162	200	200	200
benzene	0.305	194	171	150
naphthalene	0.383	192	176	136
anthracene	0.410	191	159	132

is a poor parameter for characterizing the three catalyst surfaces. Considering a complex mixture of reactants (such as hydrogen, benzene, naphthalene and anthracene) it is possible to choose a catalyst that has relatively more surface accessible to anthracene, for example, by choosing the catalyst with the lowest surface fractal dimension. The underlying assumption, of course, is that the active sites are evenly distributed throughout the catalyst surface.

For catalytic hydrocracking then, the catalyst with the lowest surface fractal dimension (assuming equivalent N₂ BET areas) should present the highest accessible area for asphaltenes. Hydroprocessing catalysts are often described as sponges or as porous solids with very high "internal" surface as opposed to "external" surface. High "internal" surface is ascribed to a pore structure where the classical mathematical model of a pore is a cylinder with smooth walls. This model may be described by a Menger sponge model [1,5]. The alternate picture of these materials is as a very rugged surface which is space-filling to a degree described quantitatively by a surface fractal dimension. The relationship between surface fractal dimension, D , and average cylinder-equivalent pore diameter has been explored [6]. The surface fractal dimension, D , is clearly a useful quantitative parameter for surface characterization.

An interesting catalyst has been described for the ASVAHL hydrodemetallization (HDM) process [7]. This is a burr-shaped catalyst with no "internal" surface as opposed to a sponge. The branching of this burr appears to be self-similar over a range of scale. The outside of the burr would appear smooth to a large asphaltene molecule. The initial reactions of HDM and cracking occur at the outside of the catalyst particle and it is here that metals are deposited. Smaller

Table 2
adsorbate

adsorbate	Calculated N ₂ BET surface area (m ² g ⁻¹)		
	$D = 2.10$	$D = 2.50$	$D = 2.90$
anthracene	100	100	100
nitrogen	105	126	152

molecules penetrate the burr where further reactions may occur. The entire catalyst then would appear to open up to expose new surface to geometrically smaller molecules. In describing this catalyst as a porous material, one would model it as a solid with pore sizes ranging from very large at the outside edges to small in the center of the burr.

Equation (1) quantifies the effect of particle size on apparent surface area. For a high D particle, the apparent surface area is independent of R . For particles of intermediate surface fractal dimension (such as most transition metal oxides), this equation gains importance as it does in fine particle science [8]. Nitrogen BET data for microporous materials should be treated with caution. Applications of fractal geometry in adsorption studies on microporous petroleum coke have been examined [8b].

3. Reaction dimension

The numerous parameters which dictate the chemical reactivity of a fractal boundary may be described by an empirical scaling exponent, D_R the reactive surface fractal dimension. This can be interpreted as the effective fractal dimension of an interface towards reaction. It has been demonstrated [9] that the initial rate of reaction, v , with the surface of a particle i.e., thermal decomposition or gasification is related to particle size by:

$$v = k_3 R^{D_R-3}. \quad (3)$$

The reactive surface fractal dimension is a measure of the activity of the reactive surface which is a sub-set of the total particle surface. Farin and Avnir have reviewed several examples of eq. (3) and discussed the relationship between D_R and D [9]. Equation (3) should also find application in heterogeneous catalytic reactions.

The catalytic activity of metal catalysts dispersed on high surface area supports has been shown [10] to exhibit similar scaling behaviour:

$$a = k_4 R_p^{D_R} (\text{mol s}^{-1} \text{ per particle}) \quad (4)$$

$$a = k_5 R_p^{D_R-2} (\text{mol s}^{-1} \text{ per exposed surface site}) \quad (5)$$

$$a_g = k_6 R_p^{D_R-3} (\text{mol s}^{-1} \text{ g}^{-1}). \quad (6)$$

In eqs. (4) to (6), R_p represents the radius of the metal particles on the support and D_R is the reaction dimension. The reaction dimension provides a quantitative measure of structure sensitivity. Farin and Avnir [10] have noted a range of values from $D_R = 0.4$ to $D_R = 6$. The reaction dimension is affected not only by specific molecule/metal interactions but also by the support morphology.

When catalytic activity per exposed surface atom is independent of metal crystallite size, the reaction is structure insensitive. This occurs when $D_R = 2$, eq.

(5). In terms of activity per particle, eq. (4), the activity scales with R^2 . Therefore, all surface atoms contribute equally to catalytic activity regardless of crystal plane. The reaction dimension is easily determined from log-log plots of eqs. (4), (5) or (6). The real value of D_R , however, occurs when specific active site populations can be assigned to D_R values. The easiest specific sites to visualize may be corners, edges, and planes. Where D_R is less than 2 and the surface of the metal crystallite has dimension 2, a subset of active sites, n_s , exists which grows slower than the total number of surface sites, n_s . The opposite case, D_R greater than 2, means that the subset of active sites grows faster than the total number of surface sites. The performance of this particle size scaling analysis indicates that if the particle is magnified by a factor of N , then a total of N^D features appear.

4. Applications of reaction dimension

A great deal of published literature can be examined to demonstrate a scaling analysis of typical Mo/Al₂O₃-catalysts. The rate of hydrodesulphurization (HDS), for example, may be related to the effects of molybdenum loading. Where eq. (6) relates catalytic activity to metal crystallite size in supported catalysts, it is perhaps easier to relate HDS activity to molybdenum loading for hydrotreating catalysts. The data of Okamoto et al. [11] are plotted in fig. 1 for thiophene HDS. This is a log-log plot of thiophene conversion (400°C, atmospheric pressure) against molybdenum loading. The loading has been expressed as the number of molybdenum atoms per square nanometer of N₂ BET surface area. This unit of loading was chosen as a better approximation of surface site density to facilitate comparisons of different alumina supported catalysts. Figure 1 exhibits regions of structure sensitivity for thiophene HDS above and below a molybdenum loading of 2.7 Mo nm⁻². The reaction dimensions for the two linear regions calculated from the slope of the log-log plot using eq. (6) are 5.2 and 3.7 for the low and high loadings.

Similarly, the data of Thomas et al. [12] for thiophene HDS (400°C, atmospheric) are presented in fig. 2. These data were generated to observe the effects of impregnation methods (i.e., wet and dry) on catalyst activity. Clearly, when plotted in terms of m^3 thiophene converted per gram-catalyst second, the various preparation techniques produce final catalysts with the same structure sensitivity. The reaction dimension, D_R , determined from these data is 4.5 below a loading of 2.7 Mo nm⁻² and 3.4 above. Bachelier et al. [13] have examined the effect of molybdenum loading on thiophene HDS (420°C, atmospheric) and on oxygen sorption at 60°C. Catalysts were prepared by a normal aqueous impregnation of gamma alumina using ammonium heptamolybdate. The data are shown in fig. 3 as a log-log plot of reaction rate (mol g⁻¹ h⁻¹) or oxygen adsorption (μmol g⁻¹) against loading. Two linear regions were again observed. For thiophene HDS, a reaction dimension of 5.2 is calculated for loadings below 2 Mo nm⁻² and 3.7 at

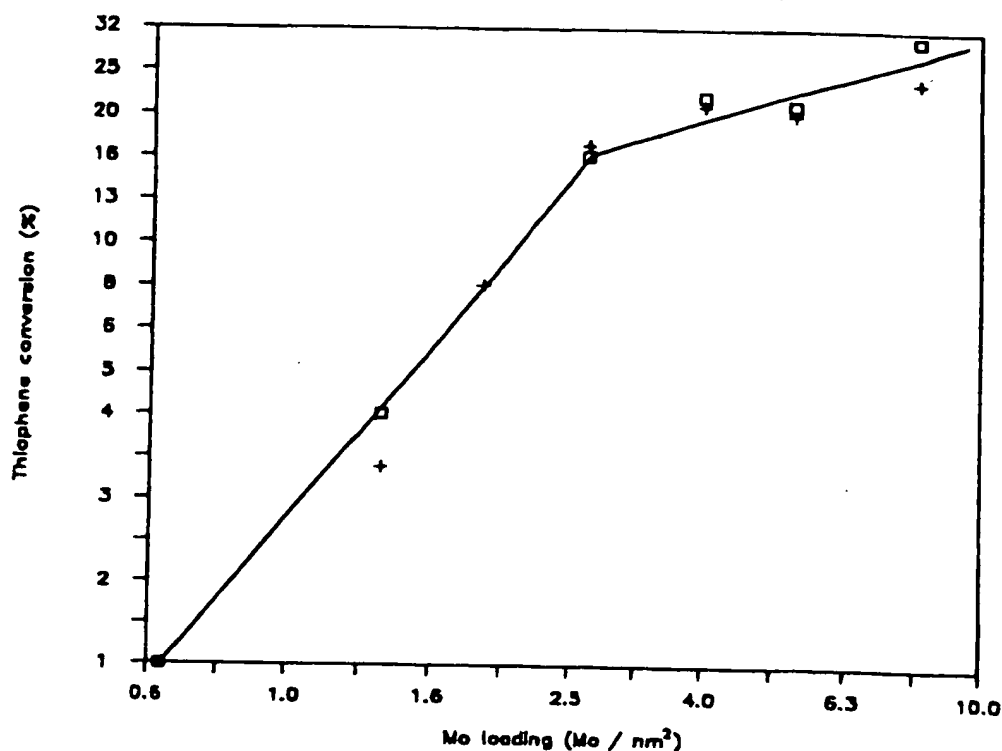


Fig. 1. The conversion of thiophene over a series of Mo/Al₂O₃ catalysts; □, ref. [11a]; +, ref. [11b].

higher loadings. The oxygen adsorption data followed similar trends with calculated reaction dimensions of 5.0 and 3.2 for the low and high loadings, respectively.

The three examples demonstrate that the structure sensitivity of thiophene HDS can be quantified by a reaction dimension, D_R . In all cases, there is a change in structure sensitivity at molybdenum loading between 2 and 3 Mo nm⁻². It is anticipated that this point coincides with the beginning of molybdenum aggregation with increased loading.

It is apparent [14–16] that MoO₃ can be detected by laser Raman Spectroscopy (LRS) only at loadings above 3 Mo nm⁻² after calcination at 500 °C. Extended X-ray adsorption fine structure (EXAFS) indicated no evidence of MoO₃ in a catalyst of 2.4 Mo nm⁻² loading [17,18]. The EXAFS study suggest a large degree of disorder with very small amounts of crystalline material, i.e., less than 1 nm diameter. At loadings below which MoO₃ or Al₂(MoO₄)₃ are detectable by LRS or EXAFS, an interaction species has been described [14,19]. A tetrahedral coordination for molybdenum predominates at low loadings, tetrahedral and octahedral coordinations at 2.8 Mo nm⁻². An increase in both octahedral and

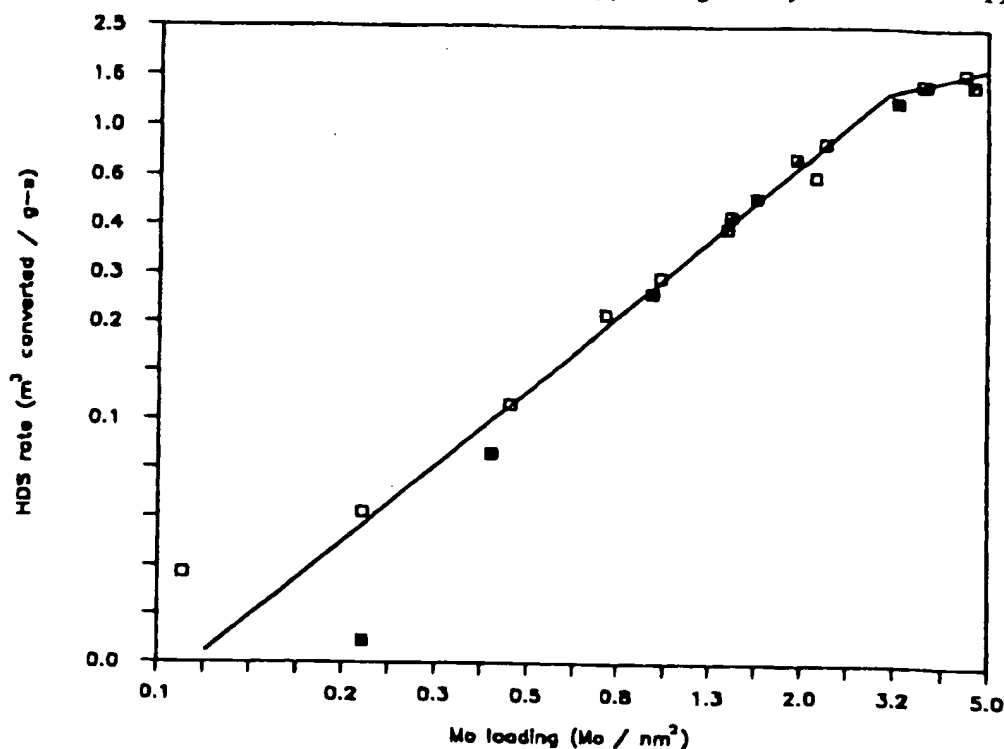


Fig. 2. The rate of thiophene HDS for a series of Mo/Al₂O₃ catalysts; □ dry impregnation; ■ wet impregnation; ◐, effect of pH, ◑, boehmite; ref. [12].

tetrahedral molybdenum with increased loading was observed [14]. A maximum in tetrahedral coordination occurred at 1.7 Mo nm⁻² and in octahedral at 4.5 Mo nm⁻² loadings. Tetrahedral molybdenum was thought to occur in isolation, i.e., well-dispersed whereas octahedral molybdenum was thought to exist in association with other Mo groups.

The data presented in the figures clearly describe an empirical scaling phenomenon. The application of a fractal descriptor, D_R , results in a quantitative description of catalyst structure sensitivity. This is useful in comparing catalysts prepared by different methods using various alumina supports. In addition, there is evidence to suggest that the molybdenum loading may be related to molybdenum dispersion, aggregation, or the size of ordered regions on the catalyst surface. There may be examples in the literature where rates of reaction for a series of reactants are presented. In some cases it has been stated that large molecules react at a lower rate than small molecules due to steric hindrance. The reaction rates are most often presented as moles per gram or moles per m² N₂ BET surface area. As indicated in tables 1 and 2 however, large molecules simply do

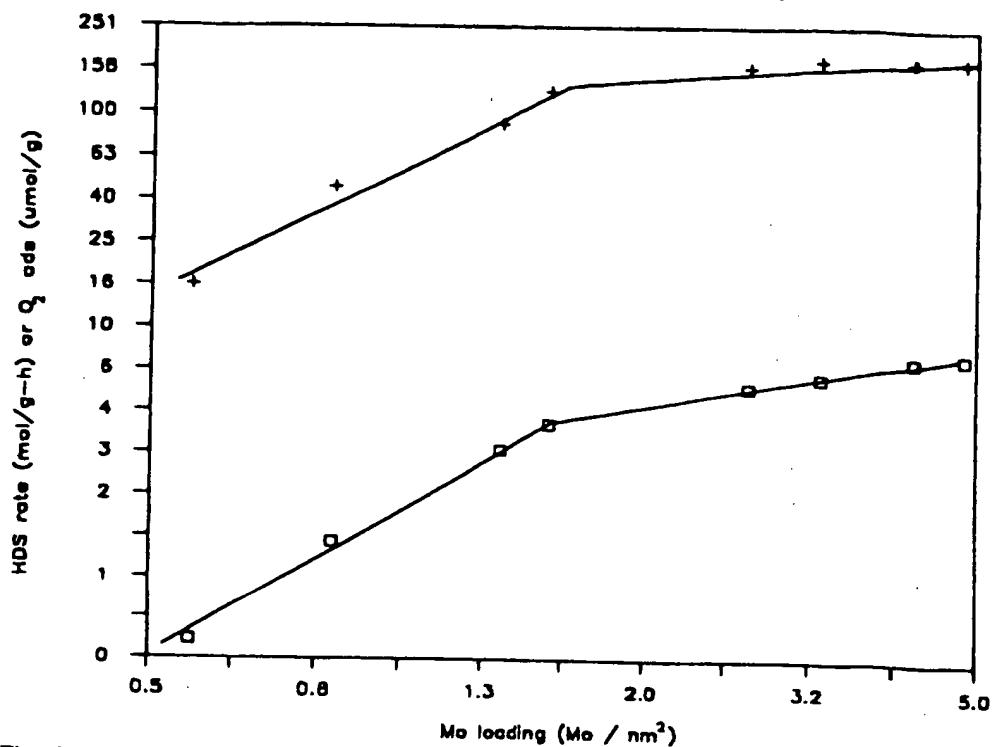


Fig. 3. Thiophene HDS activity, \square and oxygen chemisorption capacity, $+$, for a series of $\text{Mo}/\text{Al}_2\text{O}_3$ catalysts; ref. [13].

not "see" the same quantity of surface as small molecules. Where rate is controlled by molecular/surface geometry, the initial rate of reaction is controlled by the effective reactant cross-sectional area, a_m :

$$V = k_1 a_m^{-D_R/2} \quad (7)$$

In this example, a log-log plot of rate of reaction against reactant cross-sectional area would give a straight line of slope $-D_R/2$.

Wilson et al. [20] present data for the hydrogenation of a synthetic crude middle distillate over a commercial $\text{Mo-Ni}/\text{Al}_2\text{O}_3$ hydrotreating catalyst. The feed and products were accurately characterized in terms of alkylbenzene, benzocycloparaffin and benzodicycloparaffin fractions. The rate of hydrogenation obviously decreased with increased reactant size. When plotted according to eq. (7), the data indicate a reasonable relationship, as shown in fig. 4. The effective cross-sectional areas of fractions were approximated as before [4] using benzene, tetralin, and octanthrene as model reactants. In spite of the approximations in the rate measurements and estimates for a_m , the trend is apparent. In this discussion, the scaling parameter is the size of the reactant molecule. The measured reaction

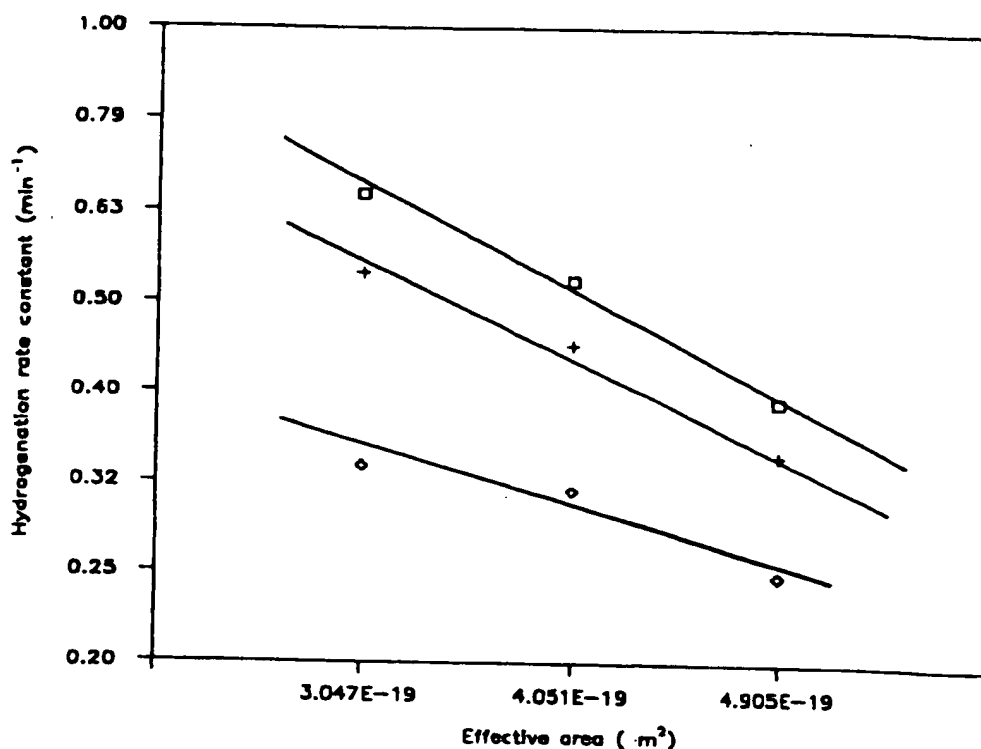


Fig. 4. The rate of hydrogenation as a function of reactant size for hydroprocessing a synthetic crude distillate over Mo-Ni/ Al_2O_3 ; \square , 380 °C; +, 360 °C; \diamond , 340 °C; ref. [20].

dimension, $D_k = 2$, suggests that the reaction is not structure-sensitive with respect to reactant size. The catalyst, therefore, is equally accessible to all three molecules for hydrogenation. Since the accessible surface area varies with adsorbate size for a porous catalyst, eq. (2), the conclusion is that catalyst reactivity towards hydrogenation occurs only on the external parts of the catalyst. Similar scaling analyses for other reactions such as hydrodesulphurization, hydrodenitrogenation, hydrodemetallization or asphaltene conversion would provide useful information on the structural sensitivity of these important reactions.

5. Conclusions

The properties of typical hydroprocessing catalysts have been discussed from the standpoint of fractal geometry. The potential of the fractal approach for characterizing catalysts and catalytic reactions has been demonstrated. The principal conclusion is that hydroprocessing catalysts are more accurately quantified by surface fractal dimension, D , rather than by N_2 BET. Equations relating

the apparent surface area to particle size and adsorbate cross-sectional area are also appropriate for characterizing hydrotreating catalysts. The concept of a reaction dimension appears to be a promising parameter for characterizing the reactivity of heterogeneous catalytic systems.

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Characterization of fractal surface roughness and its influence on diffusion and reaction

Marc-Olivier Coppens *

Delft Department of Chemical Technology, Delft University of Technology, Julianalaan 136, 2628 BL Delft, The Netherlands

Abstract

To investigate the effect of surface roughness on diffusion and reaction in porous 'amorphous' catalysts, a realistic model of roughness is necessary. By combining small-angle and wide-angle X-ray scattering, the suggestion from adsorption experiments that the surface is often fractal can be confirmed, since these techniques allow to measure the surface and bulk properties over a wider range of scales, so that the complete scaling regime, if present, can be revealed. The fractal dimension can be determined, as well as the inner and outer cutoff of the fractal scaling regime. No significant fractal surface roughness is found for zeolites, but is shown for such materials as a mesoporous γ - Al_2O_3 , catalytic reforming and hydrotreating catalysts. Results from the simulation of aggregation phenomena similar to those occurring during the sol-gel synthesis used in catalyst preparation lead to additional insights. The fractal surface roughness of a catalyst or catalyst support on molecular scales has a significant influence on the conversions and selectivities of chemical reactions, especially when they are limited by Knudsen diffusion. This effect is felt up to the scale of industrial reactors, which implies that changing the fractal surface roughness can improve the performance of an industrial process. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Small-angle X-ray scattering; Fractal; Porous catalyst; Diffusion; Reaction

1. Introduction

Recent years have seen an increased use of zeolites as catalysts, catalyst supports, or for separations [1–4]. Mesoporous sieves such as MCM-41 are extending the range of controlled pore structures into the mesopore regime and beyond [5,6]. Nano-controlling reactions through an imposed pore network architecture is one of the

main reasons driving this research. Nevertheless, cheap disordered amorphous mesoporous catalysts and catalyst supports are still most frequently used in the chemical industry [2–4]. They are also not as 'amorphous' as their etymology suggests, since their surface or pore volume may contain an internal symmetry as well. Characterizing this internal symmetry — self-similarity — and studying its influence in catalysis, is the object of this paper.

Zeolites and M41S periodic mesoporous silicas obey a translational symmetry, i.e. there are repeating units in one, two or three dimensions.

* Tel.: +31-15-2784399; fax: +31-15-2784452.

E-mail address: m.o.coppens@tnw.tudelft.nl (M.-O. Coppens).

Pfeifer and Avnir's pioneering work in the eighties [7–9] demonstrated the possibility for the surface of many 'amorphous' porous materials to obey another internal symmetry, that had been proposed earlier by Mandelbrot [10] as a remarkably universal symmetry in nature, that of fractal self-similarity. Through the adsorption of molecules of different sizes, acting as probes of surface roughness, Avnir and Pfeifer [7–9] showed that in many cases, the internal surface area S of porous materials is size-dependent in a particular way: it is a power law of the molecular probe size δ , i.e. $S \sim \delta^{2-D}$, where D lies between 2 and 3, both limits included. This was interpreted as being a result of the tortuous nature of the surface, very similar to a natural coastline, as Adamson [11] already intuitively noted: large fjords or irregularities along the surface are bordered by smaller ones, and even smaller fjords border the latter in a similar way, and so on, from a largest scale (the outer cutoff) to a smallest (the inner cutoff) [7–9]. This is schematically shown in Fig. 1. This invariance under magnification is typical for fractals [10]. The exponent D , the fractal dimension, is a measure of the space-filling capacity of the surface; it is 2 for a Euclidean surface, such as the smooth surface of graphite, and it can be as high as 3 for the space-filling surface of some silica or alumina gels. Mandelbrot's [10] self-similarity of coastlines and other meso- and macroscopic shapes was thus extended into the molecular range.

The results of Pfeifer and Avnir imply that, if the surface is fractal on molecular scales, the surface area measured by nitrogen adsorption, the most commonly used technique, is insufficient, in view of the fact that in many chemical reactions or sorption processes using these same porous materials, the species have a very different size. To which extent it is insufficient can be seen from simulation results, as presented in the next section.

A lot of work has since concentrated on the characterization of molecular fractal surface roughness of porous materials [12–16]. One of the most frequently applied techniques has been adsorption measurements using different probes. It was quickly recognized, however, that this technique has its limitations, as is shortly reviewed in the next section. However, alternatives bypassing these limitations exist, one of them being Neimark's highly practical thermodynamic method [17–19], which can be applied to a conventional nitrogen adsorption/desorption experiment. Another powerful alternative is to combine small-angle and wide-angle X-ray scattering (SAXS/WAXS), which is the technique used in this paper. The internal surface roughness on molecular scales can also be probed by NMR [20], and using multilayer adsorption [21–23], amongst others [12]. Because of the less straightforward interpretation of the results, the latter techniques are preferably used in conjunction with one of the former.

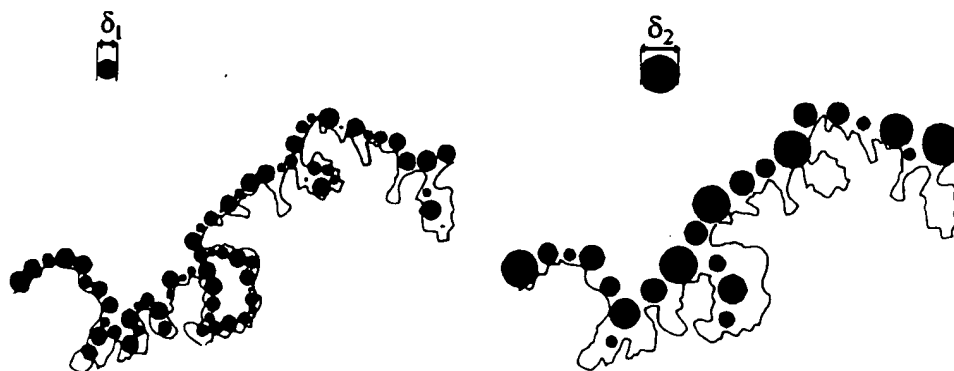


Fig. 1. Schematic representation of monolayer adsorption on the fractal surface of a catalyst pore. The small molecules on the left have access to a larger surface than the large molecules on the right.

A recent paper by the author reviews the effect of surface roughness on diffusion and reaction in porous catalysts [15]. Some of the conclusions will be repeated here, since they show the potential of fractal models to not only perform reaction engineering calculations, but also, by tuning the geometrical properties of the surface, to control conversions and selectivities of chemical processes. First, attention will be paid to the fractal surface characterization of porous catalysts using SAXS/WAXS.

2. Characterization of the surface roughness of porous catalysts

To investigate the geometrical heterogeneity of the surface of porous catalysts on molecular scales, several techniques are available, the principal of which were mentioned in the introduction. Monolayer adsorption of molecules with a different size δ is an elegant technique that has first indicated the possible fractality of the rough surface of many porous catalysts. The number of molecules in a monolayer on a fractally rough self-similar surface scales like $N \sim \delta^{-D}$, so that the surface area should scale like $S \sim \delta^{2-D}$ for a self-similar surface with fractal (adsorption) dimension D . However, there are some disadvantages to this method as well [15–17]. First, it is not easy to carry out a series of experiments with molecular probes with a sufficiently differing size, so that power law scaling can only be checked within a limited range. The use of very large molecules, such as polymers, could extend the range of investigation, but is often cumbersome and the question is shifted to a correct representation of the conformation of the adsorbed molecules. Checking power law scaling within a narrow range of data, say less than a decade, is dangerous; values different from 2 or 3 may be too quickly interpreted as being a result of surface irregularity, since the statistics are not sufficiently accurate. In addition, if the surface is indeed fractal, its scaling regime can rarely be obtained. Finding the scaling regime is useful for practical applications in, e.g. catalysis, and to help interpreting the results. A second problem with ad-

sorption measurements is the possibility of different chemical interactions between different probe molecules and the surface. In that case, the results are a reflection of chemical, rather than geometrical heterogeneity, or a mixture of both. Separating the effects of different types of heterogeneities is difficult [24,25].

Nevertheless, adsorption methods using a single probe, typically nitrogen, can be used to investigate surface roughness. Pfeifer and Avnir first proposed to compare adsorption measurements carried out on particles of different sizes, to explore how the specific surface area, measured with, say, nitrogen, scales with particle size R . A fractal self-similar surface with dimension D would lead to the scaling law $S \sim R^{D-3}$. However, this result is only valid if the particles are formed through some self-similar process leading to an outer cutoff that is proportional to R as well. Neimark introduced an easy to use method based on capillary condensation of the inert nitrogen on a fractal surface, for which $S \sim a_c^{2-D}$, where a_c is the mean radius of curvature. The latter is related to the relative pressure P/P_0 through the Kelvin equation, while S at any relative pressure can be found by integration of the isotherm from the current value to the maximum value for $P \rightarrow P_0$ according to the Kiselev equation [17–19]. In fact, the method is quite similar to porosimetry, since it is applied to adsorption in the pore-filling regime. This thermodynamic method can be used for mesopore irregularities larger than 1–2 nm.

An alternative method to adsorption, as already indicated in the introduction, is small-angle X-ray scattering (SAXS). This is a useful alternative that can provide interesting information over a wide range of length scales, and which is a purely physical technique, not prone to network hysteresis effects or energetic effects that may affect adsorption methods. For an introduction to SAXS, see [26–28]. The intensity I of an X-ray beam, scattered by the sample at the same wavelength λ as the source, is measured as a function of the scattering angle θ . The scattering is a result of the position dependence of the electron density. The intensity I measured as a function of the length of the scattered wave vector, $q = 4\pi/\lambda$

$\sin(\theta/2)$, yields information about structural (or, actually, electron density) correlations on scales $\delta \sim 1/q$ (viz. Bragg's law). Because the angles at which the measurements are performed with a SAXS apparatus are much smaller than with XRD (down to a few minutes), information on colloidal scales or scales between about 1 and 100 nm (sometimes even larger) can typically be obtained. Crossovers and features of a specific size in this range can be measured with SAXS, which is, therefore, popular in polymer science, and for the measurement of the size of micelles and colloidal particles. It has also been used for the determination of particle size (distributions) in catalysis, by filling the pores with an electron density matching liquid, to avoid scattering at the pore surface [29,30]. However, also pore size distributions and surface roughness can be conveniently probed. In this context, it is useful to remember that fractality is a symmetry, leading to specific power-law correlations. Through scattering techniques, these correlations are measured in the Fourier domain, where they also lead to power laws. A nice overview of the application of small-angle scattering to fractal morphological investigations is given by Schmidt [31,32]. For a self-similar surface fractal, Bale and Schmidt [33] showed that $I \sim q^{D-6}$, which is an extension of Porod's $I \sim q^{-4}$ law for smooth surfaces. To derive this equation, they used a two-phase approximation: the porous material consists of two phases with a constant electron density, and the interface is a self-similar fractal. In addition, the solid is assumed to be representable by a set of rigid solid spheres. Apart from a vast literature on fractal aggregates [34,35], several solid materials were tested using SAXS (and SANS, a similar technique using neutrons), such as porous rocks [14], Vycor porous and controlled-pore glass [36], as well as silica xerogels and coal particles [37], to give a few examples. The technique seems equally applicable to the industrial mesoporous catalysts, the problem of interest to this paper.

One potential drawback of scattering methods is that the investigated surface of a porous material is not necessarily the surface accessible from the outside, i.e. the surface accessible by diffusing, adsorbing and/or reacting molecules. Part of the

pore surface may indeed be occluded. The way in which the pores and their surface are formed should indicate whether inaccessible pores constitute an important part of the material and whether the inaccessible and accessible surface have different morphologies. In case of doubt, density matching liquid pore filling can be used to separately study the occluded pores, a technique especially useful to study porous carbons. This was not done for the catalysts studied here, because their sol-gel based synthesis should not lead to a significant occluded porosity or to a different surface morphology of occluded and externally accessible surface; the reaction studies in the next section can, therefore, make use of the (fractal) surface properties derived in this section.

The focus here is on a number of mesoporous alumina supported catalysts, used in refinery and petrochemical processes. Results for a PtRe/Al₂O₃ catalyst used in the catalytic reforming of naphtha are shown in Fig. 2 by way of example. This figure combines results obtained with three different apparatus, to cover a range of scales going from Ångströms to about 50 nm. Results for the largest scales were obtained at very small angles, using synchrotron radiation at the Institut Laue-Langevin in Grenoble — the downward deviation at the smallest angles is a result of the beam stop, which is blocking the (overpowering) radiation passing straight through the material. The data at average scales were obtained using X-rays from the synchrotron in Daresbury. Finally, the data at the smallest scales, corresponding to the largest angles, cannot be obtained by SAXS, but were acquired using wide-angle X-ray scattering (WAXS) in the Shell Research and Technology Center in Amsterdam. A nice mutual overlap of the results can be observed, covering an impressive 6–7 orders of magnitude in intensity. By using WAXS, the for catalysis so interesting molecular range can even be probed. A clear power-law scaling is seen in a relatively broad regime; the inner and outer cutoff of the scaling regime can easily be calculated from the knees in the curve, $\delta_{\min} \sim 1/q_{\max}$ and $\delta_{\max} \sim \pi/q_{\min}$ [31]. The smallest scale is indeed seen to be of the order of very small molecules, a few Ångströms in size, while the largest scale is similar to the average

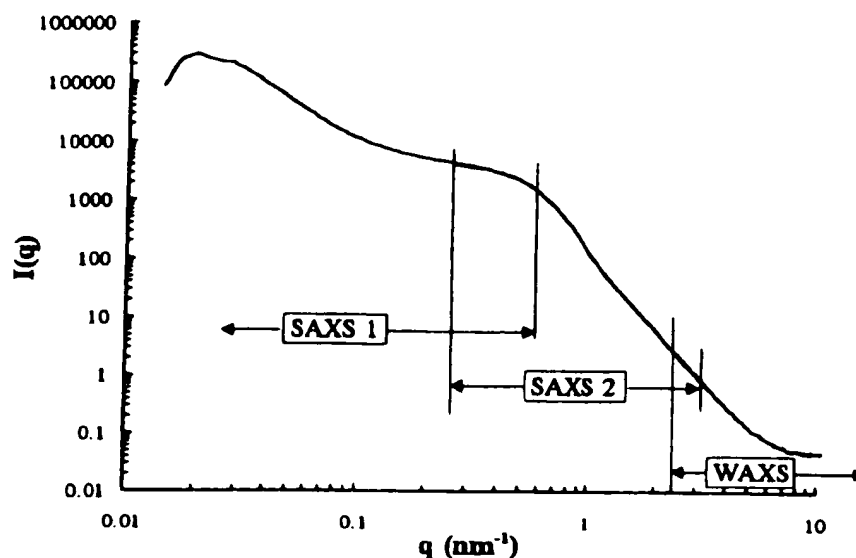


Fig. 2. SAXS/WAXS measurement results for a PtRe/Al₂O₃ catalytic reforming catalyst.

mesopore size of this material and the size of the aggregates it consists of, ~ 6 nm. The results also confirm those obtained for another reforming catalyst within a narrower regime, using a Kratky camera with a Cu-K α X-ray source. A pretreated, presulphided catalyst that has seen the reactor feed, gives similar results. The Pt and Re content of the catalyst are 0.3 wt.% each, and it can be verified that such a small content has very little effect on the results (note that the particle size can be found using electron density matching, as mentioned earlier [29,30]). All this points toward a consistent measurement of the geometrical surface characteristics of the catalyst.

Surprising was the absolute value of the slope in the scaling regime, however, which was found to be 4.33 with high accuracy. This is significantly larger than 4, corresponding to a smooth surface (Porod's law), and represents a very steep decrease of the intensity with $q \sim 1/\delta$. A value smaller than 3 would have corresponded to a mass or volume fractal ($I \sim q^{-D}$) [31,32], while a value between 3 and 4 is traditionally attributed to a fractal surface, using Bale and Schmidt's expression $I \sim q^{D-6}$. Values larger than 4 have rarely been reported. Experiments with CoMo/Al₂O₃ and NiMoP/Al₂O₃ hydrotreating catalysts led to slightly different values of the slope and cutoffs, but a very similar behavior with again a

slope larger than 4. An alumina support led to an even higher slope of 4.6, again using mutually corroborating, reproducible SAXS and WAXS results.

Fig. 3 shows the scattering results for a Pt-ultrastable Y faujasite used for hydrocracking of gasoil. Zeolites like faujasite are crystalline aluminosilicates, in contrast to the amorphous mesoporous materials investigated earlier. The dealumination of faujasite by steaming leads to the formation of mesopores. Their size of around 3 nm (knee at $q \sim 1$ nm⁻¹ in the SAXS/WAXS) nicely coincides with a typical value mentioned in the literature for cages in this catalyst [38]. The slope for $q > 1$ nm⁻¹ is 4.0, consistent with Porod's law for non-fractal surfaces.

To find an explanation for the origin of the power larger than 4 for the mesoporous aluminas, the origin of Bale and Schmidt's scaling law should be recalled. For such materials, the two-phase model could be an oversimplification. A representation of the alumina as consisting of a collection of spherical aggregates with fractal surface roughness up to the order of the size of the aggregates themselves (as observed) implies a gradual power-law decay, rather than a sudden drop of the density from the center of the aggregate to its outside. In this context, it is interesting to mention that scaling with a power larger than

4 was also found by Schaefer [39] for surfaces covered with a tensio-active compound, and by Schmidt et al. [40] for reversed phase silicas with grafted alkane layers that have a density dropping as a power law with the distance to the silica surface. A more refined analysis again leads to a power larger than 4. Moreover, based on a solid-on-solid model of surface roughness, a detailed derivation by Wong [41] led to a law $I \sim q^{2+D}$ for certain fractally rough porous media, corresponding to powers between 4 and 5, as also seen in the experiments presented here. Further investigation of this interesting fractal scaling is underway.

It should be stressed that the fractal characterization should always, whenever possible, be done with the source or preparation of the material in mind. Many mesoporous amorphous catalysts and supports are prepared through a series of steps that starts with a sol–gel synthesis. Aggregation in solution, far from equilibrium, often leads to fractal structures or particles with a fractal surface. This is shown both from experiments and simulations [34]. Subsequent filtering, drying and calcination may modify the texture and surface structure, and generally densify the particles. Also electron microscopy images frequently reveal a rough, disordered structure. A fractal surface within a finite scaling regime, corresponding to

the sizes of the elementary particles and the aggregates, is, therefore, a good possibility, which may then be tested by the described methods.

3. Effect on diffusion and reaction

In chemical reactions catalyzed by a porous (supported) catalyst, molecules diffuse through the pore space, collide with its walls, and react on the surface [2,4,42]. Molecular scale fractal surface roughness of the internal catalyst surface may therefore, have an influence on diffusion and reaction phenomena.

First, it influences the surface area available to reactions occurring on the fractal surface [12]. The effect of a fractal surface morphology on molecular diffusion toward this surface, and reaction on it, has been studied by several authors [43–47]. A more detailed list of references is included in [45,48,15].

Second, it influences the Knudsen diffusivity, frequently the dominating diffusion mechanism for gas phase reactions in mesoporous catalysts [42,49]; since many reactions of industrial relevance are diffusion limited, this influence translates into an effect on conversions and selectivities [42]. Knudsen diffusion is the dominating diffu-

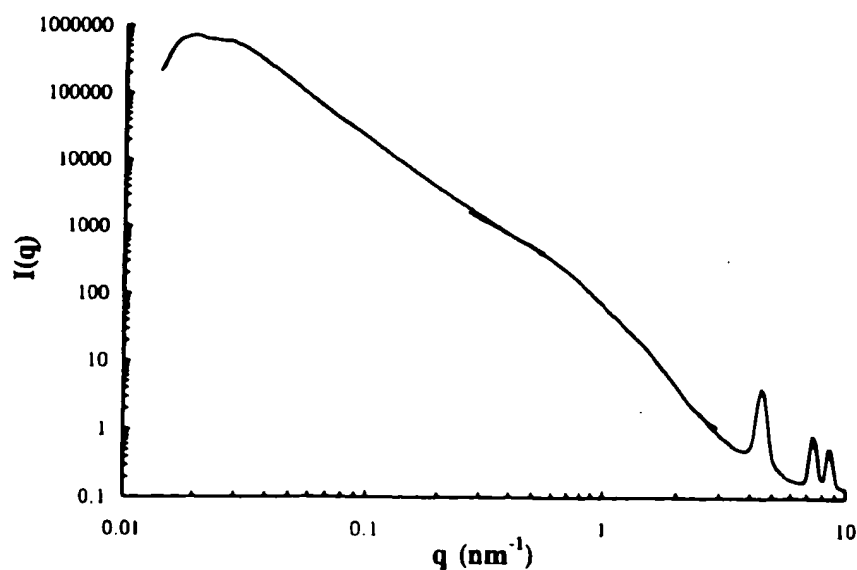


Fig. 3. SAXS/WAXS measurement results for an ultrastable faujasite Y, used for hydrocracking of gasoil.

sion mechanism when the mean free path of the gas molecules is of the same order of magnitude or larger than the pore size. In that case, collisions of the molecules with the walls are more frequent than intermolecular collisions. The diffusivity can thus be expected to be influenced by the surface morphology. A light molecule diffuses more quickly than a heavy molecule, but is usually also smaller. If the roughness is minor compared with the pore size, the size effect will be small [50,51], yet, if it is important, the collision frequency of the molecules with the walls of the irregularities will be significantly higher for small molecules that have access to more and smaller fjords than large molecules [15,52,53]. A mean-field approximation shows that the Knudsen diffusivity D_K is approximately inversely proportional to the accessible surface area [52], so that $D_K(\delta) \sim D_{K0} \delta'^{D-2}$ [there is a misprint in [15], equation 7], where D_{K0} is the Knudsen diffusivity in a smooth pore and δ' is the effective diameter of the molecules δ divided by the outer cutoff of the fractal scaling regime, as measured by, e.g. SAXS. More detailed calculations, based on a first-passage time calculation, lead to a two-parameter equation $D_K(\delta) \sim D_{K0} / [1 + \alpha(1 - \delta'^\beta)]$, where α and β can be expressed as a function of the fractal dimension of the surface, D , and a second parameter, the 'return probability', which depends on the shape of the fjords or irregularities [53,54,15].

Because of the dependence of the Knudsen diffusivities and the accessible surface area on molecular size, fractal surface roughness has an important effect on diffusion limited reactions. Models to calculate this influence are presented in [52,55,56] and summarized in [15]. The significance of the fractal roughness effect can be demonstrated for the case of an industrial four-reactor unit for the catalytic reforming of naphtha, a process used to increase the octane number of gasoline. The calculations are based on a reaction network that consists of 86 reactions between 29 component lumps, and includes a detailed description of multi-component diffusion inside the porous catalyst pellets, using the Stefan–Maxwell based dusty gas equations [49,42] with all binary molecular diffusivities and fractal roughness corrected Knudsen diffusivities. Simulations of diffu-

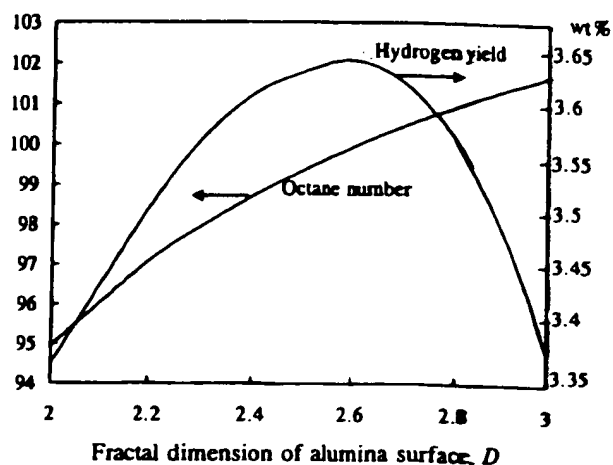


Fig. 4. Octane number of the gasoline leaving an industrial catalytic reformer, as a function of the fractal dimension of the internal surface of the PtRe/Al₂O₃ catalyst. The hydrogen yield at the outlet of the reformer is shown on the same graph. The results indicate that a further increase of the octane number at very high fractal dimensions is accompanied by excessive, undesirable hydrocracking and hydrogenolysis.

sion and reaction inside the pellets are performed all along the axis of the four fixed bed reactors in series. The octane number of the gasoline increases thanks to aromatizations and branching isomerizations. Only the ultimate result of the detailed calculations is given in Fig. 4; for more details, the reader is referred to [55,56]. Because of the higher accessible surface at higher fractal dimensions of the alumina surface, which contains acid sites catalyzing some of the reactions, the octane number steadily increases with increasing aromatization of the feed. However, the hydrogen yield peaks around $D = 2.6$, as a result of the too significant effect of undesired side-reactions involving hydrogen (hydrocracking and hydrogenolysis) when the fractal dimension of the internal catalyst surface is too high. The reason for this is the relatively higher accessibility of the rough surface to the small hydrogen molecules, so that reactions converting hydrogen become important at high fractal dimensions. The effect shows that a change in the catalyst surface morphology through a proper modification of the porous alumina synthesis may lead to an optimal increase in the octane number of the gasoline. In other words, optimization is possible by tuning the surface morphology.

4. Conclusions

It was shown how a combination of small-angle and wide-angle X-ray scattering, as an extension and alternative to adsorption studies, can be used to investigate the fractal surface morphology of industrial porous, amorphous catalysts used, e.g. in catalytic reforming and hydrotreating. This fractal roughness is in line with, but cannot directly be inferred from, the preparation of these materials. Power law scaling with a slope larger than 4 was discovered and a tentative explanation was given. The results allow to derive the complete fractal scaling regime, including inner and outer cutoffs, which is not usually possible from adsorption experiments alone. Another advantage of scattering techniques is their physical basis, independent from specific interactions between molecules and the surface or pore volume. The effect of fractal surface roughness on diffusion and reaction phenomena can be important, as was briefly shown for the example of catalytic reforming of naphtha, for which an optimal increase of the octane number and of the hydrogen yield can be predicted based on a change of the alumina fractal surface morphology.

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- [53] M.-O. Coppens, in: J. Lévy-Véhel, E. Lutton, C. Tricot (Eds.), *Fractals in Engineering*, Springer, Berlin, 1997, p. 336.
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Summary

Research Summary:

212 entries were retrieved as the result of a search of Chemical Abstracts from 1967 to July 2003 indexed under (fractal* or box(l)count*) AND catal*. 19 of these references were review articles.. There was some duplication but the following is a list of the references disclosed by the search.

Review Articles

Results

Review articles

TI Reaction engineering principles of processes **catalyzed by fractal** solids
AU Sheintuch, Moshe
CS Department of Chemical Engineering, Technion, Israel Institute of Technology, Haifa, 32000, Israel
SO Catalysis Reviews - Science and Engineering (2001), 43(3), 233-289 CODEN: CRSEC9; ISSN: 0161-4940
PB Marcel Dekker, Inc.
DT Journal; **General Review**
LA English

TI Learning from nature. **Fractals** in chemical technology
AU Coppens, Marc-Olivier
CS Chemische Technologie, Technische Universiteit Delft, Neth.
SO Natuur & Techniek Wetenschapsmagazine (2001), 69(5), 60-65 CODEN: NATWF5
PB Veen Magazines
DT Journal; **General Review**
LA Dutch

TI Theoretical study of nonlinear problems in surface chemical reaction systems
AU Xin, Houwen; Hou, Zhonghuai
CS Dep. Chemical Physics, Univ. Sci. Technology, Hefei, 230026, Peop. Rep. China
SO Huaxue Jinzhan (2000), 12(1), 1-17 CODEN: HJINEL; ISSN: 1005-281X
PB Huaxue Jinzhan Bianjibu
DT Journal; **General Review**
LA Chinese

TI Mathematics, symmetry, and chemistry. Architecture from molecules to chemical plants
AU Coppens, Marc-Olivier
CS Tech. Univ. Delft, Delft, Neth.
SO Chemisch2Weekblad (2000), 96(3), 14-15, 17 CODEN: CHWEFU; ISSN: 1389-0433
PB Ten Hagen & Stam
DT Journal; **General Review**
LA Dutch

TI Application of **fractal** in heterogeneous **catalysis**
AU Ji, Hongbing; Lin, Weiming; Wang, Lefu
CS Dep. Chem. Eng., Huanan Univ. Sci. Technol., Canton, 510641, Peop. Rep. China
SO Huaxue Tongbao (1997), (11), 21-26 CODEN: HHTPAU; ISSN: 0441-3776
PB Kexue Chubanshe
DT Journal; **General Review**

TI Analysis and control of chaotic process systems

AU Lee, J. S.; Chang, K. S.

CS ICL, AFP-Leap-Ensign Arc-Postech, Toulouse, 31078, Fr.

SO Recents Progres en Genie des Procedes (1997), 11(50, Applications des Theories du Chaos en Sciences pour l'Ingenieur), 63-84 CODEN: RPGPEX; ISSN: 1166-7478

PB Tec & Doc - Lavoisier

DT Journal; **General Review**

LA English

TI Heterogeneity of surfaces and materials, as reflected in multifractal analysis

AU Lee, Chung-Kung; Lee, Shyi-Long

CS Department Environmental Engineering, Van-Nung Institute Technology, Chungli, 32054, Taiwan

SO Heterogeneous Chemistry Reviews (1996), 3(3), 269-302 CODEN: HCREEO; ISSN: 1068-6983

PB Wiley

DT Journal; **General Review**

LA English

TI Isomorphous replacement in the zeolitic frameworks: recent advances and implications

AU Sulikowski, Bogdan

CS Institute Catalysis Surface Chemistry, Polish Academy Sciences, Krakow, 30-239, Pol.

SO Heterogeneous Chemistry Reviews (1996), 3(3), 203-268 CODEN: HCREEO; ISSN: 1068-6983

PB Wiley

DT Journal; **General Review**

LA English

TI Probing internal structures of FCC catalyst particles: From parallel bundles to fractals

AU Mann, R.; El-Nafaty, U. A.

CS Department Chemical Engineering, UMIST, Manchester, M60 1QD, UK

SO Studies in Surface Science and Catalysis (1996), 100(Catalysts in Petroleum Refining and Petrochemical Industries 1995), 355-64 CODEN: SSCTDM; ISSN: 0167-2991

PB Elsevier

DT Journal; **General Review**

LA English

TI **Fractals and catalysis**

AU Tang, Yi

CS Dep. Chem., Fudan Univ., Shanghai, 200433, Peop. Rep. China

SO Daxue Huaxue (1995), 10(6), 38-42, 48 CODEN: DAHUEW; ISSN: 1000-8438

PB Beijing Daxue Chubanshe

TI Applications of fractal theory in adsorption and catalysis

AU Dobrescu, Gianina; Vass, Mihail

CS Institute of Physical Chemistry, Roumanian Academy, Bucharest, 77208, Rom.

SO Roumanian Chemical Quarterly Reviews (1995), 3(1), 15-38 CODEN: RCQREW;
ISSN: 1221-5260

PB Editura Academiei Romane

DT Journal; **General Review**

LA English

TI Application of fractal geometry in heterogeneous catalysis

AU Guo, Xiuwei

CS Shanghai Res. Inst. Petrochem. Technol., Shanghai, 200137, Peop. Rep. China

SO Xiandai Huagong (1993), 13(4), 14-16 CODEN: HTKUDJ; ISSN: 0253-4320

DT Journal; **General Review**

LA Chinese

TI Diffusion and chemical reaction in heterogeneous gas/solid catalysis. A survey. Part 2. Pore structures; a) Simple pore models

AU Keil, Frerich

CS Inst. Chem. Reaktionstech., Tech. Univ. Hamburg-Harburg, Hamburg, D-21071, Germany

SO Chemische Technik (Leipzig, Germany) (1993), 45(6), 437-47 CODEN: CHTEAA;
ISSN: 0045-6519

DT Journal; **General Review**

LA German

TI Fractal geometry - a new approach to heterogeneous catalysis

AU Avnir, David

CS Sch. Chem., Hebrew Univ. Jerusalem, Jerusalem, 91904, Israel

SO Chemistry & Industry (London, United Kingdom) (1991), (24), 912-16 CODEN: CHINAG; ISSN: 0009-3068

DT Journal; **General Review**

LA English

TI Fractals in heterogeneous catalysis

AU Rothschild, Walter G.

CS Dep. Chem. Eng., Ford Mot. Co., Dearborn, MI, 48121-2053, USA

SO Catalysis Reviews - Science and Engineering (1991), 33(1-2), 71-107 CODEN: CRSEC9; ISSN: 0161-4940

DT Journal; **General Review**

LA English

TI Applications of **fractal geometry** for characterizing hydrotreating catalysts

AU Fairbridge, C.

CS Energy, Mines Resour. Canada, CANMET, Ottawa, ON, K1A 0G1, Can.

SO Catalysis Letters (1989), 2(4), 191-200 CODEN: CALEER; ISSN: 1011-372X

DT Journal; **General Review**

LA English

TI Fractures in colloid and interfacial chemistry

AU Moegel, Hans Joerg

CS Sekt. Chem., Martin-Luther-Univ. Halle-Wittenberg, Halle/Saale, DDR-4020, Ger. Dem. Rep.

SO Wissenschaftliche Zeitschrift - Martin-Luther-Universitaet Halle-Wittenberg, Mathematisch-Naturwissenschaftliche Reihe (1988), 37(5), 20-6 CODEN: WMHMAP; ISSN: 0043-6887

DT Journal; **General Review**

LA German

TI The **fractal** nature of molecule-surface chemical activities and physical interactions in porous materials

AU Farin, Dina; Avnir, David

CS Fritz Haber Res. Cent. Mol. Dyn., Hebrew Univ. Jerusalem, Jerusalem, 91904, Israel

SO Studies in Surface Science and Catalysis (1987), 39(Charact. Porous Solids), 421-32 CODEN: SSCTDM; ISSN: 0167-2991

DT Journal; **General Review**

LA English

TI **Catalyst** surfaces, macromolecules, and colloidal aggregates: **fractal** dimension as concealed symmetry of irregular structures

AU Pfeifer, Peter

CS Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800/1, Fed. Rep. Ger.

SO Chimia (1985), 39(5), 120-34 CODEN: CHIMAD; ISSN: 0009-4293

DT Journal; **General Review**

LA German

Review Articles

Other CAS references

TI Fractal features and catalytic performance of CeO₂/ZnO catalyst

AU He, Yong-jun; Yang, Bo-lun; Pan, Hai-min; Zhang, Chang-lei; Chen, Xuan-bing

CS Dep. Chem. Eng., Xi'an Jiaotong Univ., Xi'an Shaanxi, 710049, Peop. Rep. China

SO Shiyou Huagong (2003), 32(1), 9-13 CODEN: SHHUE8; ISSN: 1000-8144

PB Shiyou Huagong Bianjibu

DT Journal

LA Chinese

TI Changeable-dimension characterization of catalyst deposited with carbon during regeneration

AU Yang, Deming; Lin, Xiping

CS Jiangsu Petrochemical Engineering Institute, Changzhou, 213016, Peop. Rep. China

SO Huaxue Yanjiu Yu Yingyong (2003), 15(1), 51-53 CODEN: HYYIFM; ISSN: 1004-1656

PB Huaxue Yanjiu Yu Yingyong Bianjibu

DT Journal

LA Chinese

TI Silver-modified titanium dioxide thin films for efficient photodegradation of methyl orange

AU Arabatzis, I. M.; Stergiopoulos, T.; Bernard, M. C.; Labou, D.; Neophytides, S. G.; Falaras, P.

CS NCSR "Demokritos", Institute of Physical Chemistry, Athens, 153 10, Greece

SO Applied Catalysis, B: Environmental (2003), 42(2), 187-201 CODEN: ACBEE3; ISSN: 0926-3373

PB Elsevier Science B.V.

DT Journal

LA English

TI Catalyst surface at a fractal of cost - a quest for optimal catalyst loading

AU Phillips, Cynthia; Ben-Richou, Abderrahim; Ambari, Abdelhak; Fedorov, Andrei

CS G.W. Woodruff School of Mechanical Engineering, Georgia Tech., Atlanta, GA, 30332-0405, USA

SO Chemical Engineering Science (2003), 58(11), 2403-2408 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier Science Ltd.

DT Journal

LA English

Use of fractal geometry or box counting methods to describe catalysts - July 30, 2003

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Review Articles

CS College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, 310014, Peop. Rep. China

SO Chinese Journal of Chemical Engineering (2003), 11(1), 33-37 CODEN: CJCEEB; ISSN: 1004-9541

PB Chemical Industry Press

DT Journal

LA English

TI Characterizing cavity-like spaces in active-site models of zeolites

AU Torrens, F.

CS Institut Universitari de Ciencia Molecular, Universitat de Valencia, Dr. Moliner 50, Burjassot, (Valencia), E-46100, Spain

SO Computational Materials Science (2003), 27(1-2), 96-101 CODEN: CMMSEM; ISSN: 0927-0256

PB Elsevier Science B.V.

DT Journal

LA English

TI Biochips for characterizing biological processes

IN Kreimer, David I.; Nufert, Thomas H.; Ginzburg, Lev; Yevin, Oleg A.

PA Array Bioscience Corporation, USA

SO PCT Int. Appl., 150 pp. CODEN: PIXXD2

DT Patent

LA English

WO 2003042403

TI Multifractal scaling analysis of autopoisoning reactions over a rough surface

AU Chaudhari, Ajay; Yan, Ching-Cher Sanders; Lee, Shyi-Long

CS Department of Chemistry, National Chung Cheng University, ChiaYi, 621, Taiwan

SO Journal of Physics A: Mathematical and General (2003), 36(13), 3757-3772 CODEN: JPHAC5; ISSN: 0305-4470

PB Institute of Physics Publishing

DT Journal

LA English

TI Molecular Organization of Reagents in the Kinetics and **Catalysis** of Liquid-Phase Reactions: XI. Manifestation of the Structure of Solution in the Kinetics of Water Addition to Isocyanate in Water-Dioxane Mixtures

AU Tiger, R. P.; Levina, M. A.; Entelis, S. G.; Andreev, M. A.

CS Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, 117977, Russia

SO Kinetics and Catalysis (Translation of Kinetika i Kataliz) (2002), 43(5), 662-666

CODEN: KICAA8; ISSN: 0023-1584

Review Articles

LA English

TI Study on the influence of surface structure on the heterogeneous **catalytic** reaction by simulation method

AU Le, Kim Long; Lam, Ngoc Thiem; Vu, Hung Sinh

CS Fac. of Chem., College of Natural Science, Vietnam National Univ., Hanoi, Vietnam

SO Tap Chi Hoa Hoc (2002), 40(4), 43-47 CODEN: TCHHDC; ISSN: 0378-2336

PB Toa Soan Tap Chi Hoa Hoc

DT Journal

LA Vietnamese

TI Dynamic scaling of diffusion-limited reactions over **fractal** surfaces: computer simulation

AU Yan, Ching-Cher; Chaudhari, Ajay; Lee, Shyi-Long

CS Department of Chemistry, National Chung-Cheng University, Ming-Hsiung, Chia-Yi, 621, Taiwan

SO Applied Surface Science (2002), 196(1-4), 375-382 CODEN: ASUSEE; ISSN: 0169-4332

PB Elsevier Science B.V.

DT Journal

LA English

TI Granada Crystallization **Box**: a new device for protein crystallization by **counter**-diffusion techniques

AU Garcia-Ruiz, Juan Ma.; Gonzalez-Ramirez, Luis Antonio; Gavira, Jose Antonio; Otalora, Fermin

CS Laboratorio de Estudios Cristalograficos, IACT, Facultad de Ciencias, Granada, 18002, Spain

SO Acta Crystallographica, Section D: Biological Crystallography (2002), D58(10, No. 1), 1638-1642 CODEN: ABCRE6; ISSN: 0907-4449

PB Blackwell Munksgaard

DT Journal

LA English

TI Growth process for **fractal** polymer aggregates formed by perfluorooctyltriethoxysilane. Time-resolved small-angle X-ray scattering spectra and the application of the unified equation

AU Izawa, Kenichi; Ogasawara, Toshiaki; Masuda, Hideki; Okabayashi, Hirofumi; Monkenbusch, Michael; O'Connor, Charmian J.

CS Department of Applied Chemistry, Nagoya Institute of Technology, Nagoya, 466-8555, Japan

SO Colloid and Polymer Science (2002), 280(8), 725-735 CODEN: CPMSB6; ISSN: 0303-402X

PB Springer-Verlag

TI **Fractal** analysis on the structure sensitivity of gas - solid **catalytic** reaction

AU Liao, Hui; Wang, Fu-min; Xin, Feng

CS School of Chemical Engineering, Tianjin University, Tianjin, 300072, Peop. Rep. China

SO Huaxue Gongye Yu Gongcheng (Tianjin, China) (2002), 19(2), 167-171 CODEN:

HGGOER; ISSN: 1004-9533

PB Huaxue Gongye Yu Gongcheng Bianjibu

DT Journal

LA Chinese

TI **Fractal** dimension of zeolite **catalysts**

AU Torrens, Francisco

CS Institut Universitari de Ciencia Molecular, Universitat de Valencia, Valencia, E-46100, Spain

SO Molecular Physics (2002), 100(19), 3105-3109 CODEN: MOPHAM; ISSN: 0026-8976

PB Taylor & Francis Ltd.

DT Journal

LA English

TI The parameter **m** in **fractal geometry** symmetry model for isothermal diffusion reactions within porous solid **catalyst** particle

AU Duan, Yi-wen; Chen, Li-ping; Siqindalai

CS Department of Chemistry, Inner Mongolia Normal University, Huhhot, 010022, Peop. Rep. China

SO Neimenggu Shida Xuebao, Ziran Kexue (Hanwen)ban (2002), 31(2), 132-136 CODEN: NSXKEC; ISSN: 1001-8735

PB Neimenggu Shida Xuebao Bianjibu

DT Journal

LA English

TI Influence of **fractal** pore structure in Claus **catalyst** performance

AU Larraz, Rafael

CS Chemical Engineering Department, University of La Laguna, La Laguna, Tenerife, 38200, Spain

SO Chemical Engineering Journal (Amsterdam, Netherlands) (2002), 86(3), 309-317 CODEN: CMEJAJ; ISSN: 1385-8947

PB Elsevier Science B.V.

DT Journal

LA English

TI Reaction diffusion modeling in **fractal** media

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Review Articles

CS Department of Chemical Engineering, Tsinghua University, Beijing, 100084, Peop. Rep. China

SO Shiyou Huagong (2002), 31(7), 534-538 CODEN: SHHUE8; ISSN: 1000-8144

PB Shiyou Huagong Bianjibu

DT Journal

LA Chinese

TI Effectiveness factor for irregular catalyst pellet

AU Wang, Fu-Min; Xin, Feng; Liao, Hui; Li, Shao-Fen

CS School of Chemical Engineering and Technology, Tianjin University, Tianjin, 300072, Peop. Rep. China

SO Transactions of Tianjin University (2001), 7(2), 118-122 CODEN: TTUNEB; ISSN: 1006-4982

PB Tianjin University

DT Journal

LA English

TI Fractal dimension of different structural-type zeolites and of the active sites

AU Torrens, Francisco

CS Institut Universitari de Ciencia Molecular, Universitat de Valencia, Valencia, E-46100, Spain

SO Topics in Catalysis (2002), 18(3-4), 291-297 CODEN: TOCAFI; ISSN: 1022-5528

PB Kluwer Academic/Plenum Publishers

DT Journal

LA English

TI An Investigation of Submicrostructural Evolution of Freshly Precipitated ZrO₂ in Digestion for Ultrafine Sulfated ZrO₂ Catalysts by SAXS Technique

AU Zeng, Yanwei; Zhao, Yubao

CS College of Materials Science and Engineering, Nanjing University of Technology, Nanjing, 210009, Peop. Rep. China

SO Journal of Colloid and Interface Science (2002), 247(1), 100-106 CODEN: JCISA5; ISSN: 0021-9797

PB Academic Press

DT Journal

LA English

TI Morphological evolution of the aggregates in the premixed flat flame aerosol reactor

AU Chang, Hankwon; Lee, Jeungwoo; Chang, Hyuksang

CS Environmental Aerosol Engineering Laboratory, Department of Environmental Engineering, Yeungnam University, Kyungsan, 712-749, S. Korea

SO Hwahak Konghak (2001), 39(5), 563-572 CODEN: HHKHAT; ISSN: 0304-128X

PB Korean Institute of Chemical Engineers

DT Journal

TI **Fractal** Theory for the Compensation Effect Observed in a Surface Diffusion Process Studied Using Deuteron NMR

AU Rigby, Sean P.

CS Department of Chemical Engineering, University of Bath, Claverton Down, Bath, BA2 7AY, UK

SO Langmuir (2002), 18(5), 1613-1618 CODEN: LANGD5; ISSN: 0743-7463

PB American Chemical Society

DT Journal

LA English

TI Binary collision growth of supported metal **catalyst** particles

AU Gmachowski, Lech

CS Polish Academy of Sciences, Institute of Physical Chemistry, Warsaw, 01-224, Pol.

SO Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2002), 197(1-3), 183-191 CODEN: CPEAEH; ISSN: 0927-7757

PB Elsevier Science B.V.

DT Journal

LA English

TI **Fractals** of silica aggregates

AU Li, Zhihong; Wu, Dong; Sun, Yuhang; Wang, Jun; Liu, Yi; Dong, Baozhong

CS State Key Laboratory of Coal Conversion, Chinese Academy of Sciences, Taiyuan, 030001, Peop. Rep. China

SO Studies in Surface Science and Catalysis (2001), 135(Zeolites and Mesoporous Materials at the Dawn of the 21st Century), 2326-2332 CODEN: SSCTDM; ISSN: 0167-2991

PB Elsevier Science B.V.

DT Journal; (computer optical disk)

LA English

TI Recurrence quantification analysis of spatio-temporal chaotic transient in a closed unstirred Belousov-Zhabotinskii reaction

AU Masia, Marco; Bastianoni, Simone; Rustici, Mauro

CS Dipartimento di Chimica, Universita di Sassari, Sassari, 07100, Italy

SO Physical Chemistry Chemical Physics (2001), 3(24), 5516-5520 CODEN: PPCPFQ; ISSN: 1463-9076

PB Royal Society of Chemistry

DT Journal

LA English

TI Selective Co-catalysed growth of novel MgO fishbone **fractal** nanostructures

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Review Articles

CS Physics and Environmental Sciences, School of Chemistry, University of Sussex,
Falmer, Brighton, BN1 9QJ, UK

SO Chemical Physics Letters (2001), 347(4,5,6), 337-343 CODEN: CHPLBC; ISSN: 0009-2614

PB Elsevier Science B.V.

DT Journal

LA English

TI Adsorption of etioporphyrin and Ni etioporphyrin on a **fractal** silica

AU Hill, Josephine Mary; Ng, Flora T. T.

CS Department of Chemical Engineering, University of Waterloo, Waterloo, ON, N2L 3G1, Can.

SO Canadian Journal of Chemistry (2001), 79(5/6), 817-822 CODEN: CJCHAG; ISSN: 0008-4042

PB National Research Council of Canada

DT Journal

LA English

TI Characterization of **fractal** surface roughness and its influence on diffusion and reaction

AU Coppens, M.-O.

CS Delft Department of Chemical Technology, Delft University of Technology, Delft, 2628 BL, Neth.

SO Colloids and Surfaces, A: Physicochemical and Engineering Aspects (2001), 187-188, 257-265 CODEN: CPEAEH; ISSN: 0927-7757

PB Elsevier Science B.V.

DT Journal

LA English

TI A SAXS study of kinetics of aggregation of TEOS-derived sonogels at different temperatures

AU Vollet, D. R.; Donatti, D. A.; Ibanez Ruiz, A.

CS Departamento de Fisica-IGCE, UNESP, Rio Claro(SP), 13500-970, Brazil

SO Journal of Non-Crystalline Solids (2001), 288(1-3), 81-87 CODEN: JNCSBJ; ISSN: 0022-3093

PB Elsevier Science B.V.

DT Journal

LA English

TI Experimental study on hydrolysis and concentration of tetrabutylorthostannate[Sn(oBu)₄]

AU Guo, Yu-zhong; Huang, Rui-an; Wang, Jian-hua

CS College of Materials Science & Metallurgy Engineering, Kunming University of Science and Technology, Kunming, 650093, Peop. Rep. China

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-13/47-

Review Articles

PB Cailiao Kexue Yu Gongcheng Bianjibu

DT Journal

LA Chinese

TI Statistical analysis of the **fractal** gating motions of the enzyme acetylcholinesterase

AU Shen, T. Y.; Tai, Kaihsu; McCammon, J. Andrew

CS Department of Physics, University of California, San Diego, La Jolla, CA, 92093-0365, USA

SO Physical Review E: Statistical, Nonlinear, and Soft Matter Physics (2001), 63(4-1), 041902/1-041902/6 CODEN: PRESCM

PB American Physical Society

DT Journal

LA English

TI **Fractal** dimensions of Ti-supported oxide electrodes and their electrocatalytic properties

AU Liang, Zhenhaig; Dong, Lijun; Chen, Xinguo; Sun, Yanping

CS College of Chemical Engineering and Technology, Taiyuan University of Technology, Taiyuan, 030024, Peop. Rep. China

SO Cuihua Xuebao (2001), 22(2), 148-150 CODEN: THHPD3; ISSN: 0253-9837

PB Kexue Chubanshe

DT Journal

LA Chinese

TI **Fractal** characterization of the distribution of reactive sites over a rough **catalyst** surface

AU Andrade, R. F. S.; Cajueiro, D. O.; Ferreira, C. S.

CS Instituto de Fisica, Universidade Federal da Bahia, Salvador, 40210-340, Brazil

SO Physica A: Statistical Mechanics and Its Applications (Amsterdam, Netherlands) (2001), 295(3-4), 323-332 CODEN: PHYADX; ISSN: 0378-4371

PB Elsevier Science B.V.

DT Journal

LA English

TI Research for morphology of supported polyolefin **catalyst** and its effect on polymerization activity using **fractal** theory

AU Huo, Chao; Ren, Xiao-hong; Zong, Ying-wei; Yang, Yong-rong; Rong, Shun-xi

CS Department Chemical Engineering, Zhejiang University Technology, Hangzhou, 310014, Peop. Rep. China

SO Gaoxiao Huaxue Gongcheng Xuebao (2000), 14(6), 570-576 CODEN: GHGXEG; ISSN: 1003-9015

PB Zhejiang Daxue

DT Journal

LA Chinese

TI Ethylene (co)polymerization with supported-metallocenes prepared by the sol-gel method

AU dos Santos, J. H. Z.; Uozumi, T.; Teranishi, T.; Sano, T.; Soga, K.

CS Instituto de Quimica, Universidade Federal do Rio Grande do Sul, Porto Alegre, 91500-000, Brazil

SO Polymer (2001), 42(10), 4517-4525 CODEN: POLMAG; ISSN: 0032-3861

PB Elsevier Science Ltd.

DT Journal

LA English

TI Comparative investigations on the porous structure and surface **fractal** dimension of La³⁺ and Mg²⁺-doped alumina obtained by sol-gel process

AU Jovanovic, N. N.; Novakovic, T. B.; Vukovic, Z. M.

CS IChTM Center for Catalysis and Chemical Engineering, Belgrade, YU 11000, Yugoslavia

SO Physical Chemistry 2000, Proceedings of the International Conference on Fundamental and Applied Aspects of Physical Chemistry, 5th, Belgrade, Yugoslavia, Sept. 27-29, 2000 (2000), 584-586. Editor(s): Ribnikar, Slobodan; Anic, Slobodan. Publisher: Society of Physical Chemists of Serbia, Belgrade, Yugoslavia. CODEN: 69BCCG

DT Conference

LA English

TI Kinetics of N₂O **catalytic** decomposition over three-dimensional **fractals**

AU Guo, X.-Y.; Keil, F. J.

CS State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, Peop. Rep. China

SO Chemical Physics Letters (2000), 330(3,4), 410-416 CODEN: CHPLBC; ISSN: 0009-2614

PB Elsevier Science B.V.

DT Journal

LA English

TI Application of surface **fractal** to characterization of direct coal liquefaction **catalysts**

AU Zhan, Li'an; Zhu, Jisheng; Xu, Long; Yang, Jianli; Liu, Zhenyu

CS State key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, Peop. Rep. China

SO Meitan Zhuanhua (2000), 23(3), 48-52 CODEN: MEZHE6; ISSN: 1004-4248

PB Kexue Chubanshe

DT Journal

LA Chinese

Use of fractal geometry or box counting methods to describe catalysts - July 30, 2003

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CS Institute of Catalysis, Bulgarian Academy of Science, Sofia, 1113, Bulg.
SO NATO Science Series, Series C: Mathematical and Physical Sciences (2000),
546(Metal-Ligand Interactions in Chemistry, Physics and Biology), 353-369 CODEN:
NSCMFG; ISSN: 1389-2185
PB Kluwer Academic Publishers
DT Journal
LA English

TI **Fractal** characterization of wide pore range **catalysts**. Application of Pd-Ag/SiO₂
xerogels

AU Blacher, S.; Heinrichs, B.; Sahouli, B.; Pirard, R.; Pirard, J.-P.
CS Laboratoire de Genie Chimique, Universite de Liege, Liege, B-4000, Belg.
SO Journal of Colloid and Interface Science (2000), 226(1), 123-130 CODEN: JCISA5;
ISSN: 0021-9797
PB Academic Press
DT Journal
LA English

TI Preparation and characterization of alumina and chromia cryogel-based **catalysts**

AU Kirchnerova, J.; Klvana, D.; Chaouki, J.
CS Department of Chemical Engineering, Ecole Polytechnique, Montreal, QC, Can.
SO Applied Catalysis, A: General (2000), 196(2), 191-198 CODEN: ACAGE4; ISSN: 0926-
860X
PB Elsevier Science B.V.
DT Journal
LA English

TI A light and X-ray scattering study of the acid **catalyzed** silica synthesis in the presence
of polyethylene glycol

AU Agren, P.; Counter, J.; Laggner, P.
CS Department of Physical Chemistry, Materials Research Group, Abo Akademi University,
Turku, 20500, Finland
SO Journal of Non-Crystalline Solids (2000), 261(1-3), 195-203 CODEN: JNCSBJ; ISSN:
0022-3093
PB Elsevier Science B.V.
DT Journal
LA English

TI Preparation, **fractal** surface morphology and photocatalytic properties of TiO₂ films

AU Xagas, A. P.; Androulaki, E.; Hiskia, A.; Falaras, P.
CS Institute of Physical Chemistry, NCSR, 'Demokritos', Aghia Paraskevi, Attikis, 153 10,
Greece
SO Thin Solid Films (1999), 357(2), 173-178 CODEN: THSFAP; ISSN: 0040-6090
PB Elsevier Science S.A.

TI Selectivity and Deactivation of Diffusion- Limited Reactions in a Pore- **Fractal Catalyst**.
[Erratum to document cited in CA131:162028]

AU Sheintuch, Moshe

CS Department of Chemical Engineering, Technion Israel Institute of Technology, Haifa, 32000, Israel

SO Industrial & Engineering Chemistry Research (2000), 39(1), 242 CODEN: IECRED; ISSN: 0888-5885

PB American Chemical Society

DT Journal

LA English

TI Preparation and **fractal** morphology of Ti-Mg polyethylene **catalyst**

AU Huo, Chao; Ren, Xiao-hong; Zong, Ying-wei; Liu, Bai-ping; Yang, Yong-rong; Rong, Shun-xi

CS Dep. Chem. Eng., Zhejiang Univ., Hangzhou, 310027, Peop. Rep. China

SO Shiyou Huagong (1999), 28(12), 820-823, 826 CODEN: SHHUE8; ISSN: 1000-8144

PB Shiyou Huagong Bianjibu

DT Journal

LA Chinese

TI Comments on "Mechanism Discrimination in Heterogeneous **Catalytic** Reactions: **Fractal** Analysis"

AU Zhang, Baoquan; Liu, Xiufeng

CS School of Chemical Engineering, Tianjin University, Tianjin, 300072, Peop. Rep. China

SO Industrial & Engineering Chemistry Research (2000), 39(2), 573-574 CODEN: IECRED; ISSN: 0888-5885

PB American Chemical Society

DT Journal

LA English

TI Study on apparent kinetics for reactions of changeable-dimension **fractal**-particle with fluid

AU Yang, Deming; Lin, Xiping

CS Jiangsu Petrochemical Engineering Institute, Changzhou, 213016, Peop. Rep. China

SO Shiyou Lianzhi Yu Huagong (1999), 30(11), 53-55 CODEN: SLYHEE; ISSN: 1005-2399

PB Shiyou Lianzhi Yu Huagong Zazhishe

DT Journal

LA Chinese

TI On the intermediate asymptote of diffusion-limited reactions in a **fractal** porous **catalyst**

Use of fractal geometry or box counting methods to describe catalysts - July 30, 2003

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Review Articles

CS Department of Chemical Engineering, Technion, Israel Institute of Technology, Haifa, Israel

SO Chemical Engineering Science (1999), Volume Date 2000, 55(3), 615-624 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier Science Ltd.

DT Journal

LA English

TI The effect of **fractal** surface roughness on diffusion and reaction in porous **catalysts** - from fundamentals to practical applications

AU Coppens, Marc-Olivier

CS Delft Department of Chemical Technology, Delft University of Technology, Delft, 2628 BL, Neth.

SO Catalysis Today (1999), 53(2), 225-243 CODEN: CATTEA; ISSN: 0920-5861

PB Elsevier Science B.V.

DT Journal

LA English

TI NMR and modeling studies of structural heterogeneity over several lengthscales in amorphous **catalyst** supports

AU Rigby, Sean P.

CS Syntex, Cleveland, TS23 1LB, UK

SO Catalysis Today (1999), 53(2), 207-223 CODEN: CATTEA; ISSN: 0920-5861

PB Elsevier Science B.V.

DT Journal

LA English

TI Reaction Efficiency on the Surface of a Porous **Catalyst**

AU Garza-Lopez, Roberto A.; Kozak, John J.

CS Department of Chemistry, Pomona College, Claremont, CA, 91711, USA

SO Journal of Physical Chemistry B (1999), 103(43), 9200-9204 CODEN: JPCBFK; ISSN: 1089-5647

PB American Chemical Society

DT Journal

LA English

TI Large pore size and quasi-order in polyacrylamide gels at high crosslinker content

AU Asnaghi, D.; Giglio, M.

CS Dipartimento di Fisica dell'Universita di Milano and Istituto Nazionale di Fisica della Materia, Milan, I-20133, Italy

SO Nuovo Cimento della Societa Italiana di Fisica, D: Condensed Matter, Atomic, Molecular and Chemical Physics, Fluids, Plasmas, Biophysics (1998), 20D(12bis), 2175-

2180 CODEN: NCSDDN; ISSN: 0392-6737

Review Articles

LA English

TI About surface reaction kinetics on probabilistic and **fractal** substrates

AU Moiny, F.; Dumont, Martine

CS Faculte des Sciences, Universite de Mons-Hainaut, Mons, B-7000, Belg.

SO Journal of Chemical Physics (1999), 111(10), 4743-4755 CODEN: JCPSA6; ISSN: 0021-9606

PB American Institute of Physics

DT Journal

LA English

TI The electrochemical reduction of α -nitrocumene in a protic and basic medium on large surface area (porous) electrodes: electronation- protonation or electrocatalytic hydrogenation?

AU Chan-Shing, Elisa Soazara; Boucher, Denys; Lessard, Jean

CS Centre de Recherche en Electrochimie et Electrocatalyse, Departement de Chimie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.

SO Canadian Journal of Chemistry (1999), 77(5/6), 687-694 CODEN: CJCHAG; ISSN: 0008-4042

PB National Research Council of Canada

DT Journal

LA English

TI Selectivity and Deactivation of Diffusion-Limited Reactions in a Pore- **Fractal Catalyst**

AU Sheintuch, Moshe

CS Department of Chemical Engineering, Technion Israel Institute of Technology, Haifa, 32000, Israel

SO Industrial & Engineering Chemistry Research (1999), 38(9), 3261-3269 CODEN: IECRED; ISSN: 0888-5885

PB American Chemical Society

DT Journal

LA English

TI Effect of surface **fractal** dimension on **catalytic** reactions

AU Wang, Yaquan

CS State Key Laboratory of C1 Chemical Technology, Tianjin University, Tianjin, 300072, Peop. Rep. China

SO Ranliao Huaxue Xuebao (1999), 27(2), 110-115 CODEN: RHXUD8; ISSN: 0253-2409

PB Kexue Chubanshe

DT Journal

LA Chinese

TI Area determination in **fractal** surfaces of Pt and Pt-Ru **catalysts** for methanol oxidation
AU Saffarian, H. M.; Srinivasan, R.; Chu, D.; Gilman, S.
CS Applied Physics Laboratory, The Johns Hopkins University, Laurel, MD, 20723, USA
SO Electrochimica Acta (1998), 44(8-9), 1447-1454 CODEN: ELCAAV; ISSN: 0013-4686
PB Elsevier Science Ltd.
DT Journal
LA English

TI Computational Investigations into the Potential Use of Poly(benzyl phenyl ether) Dendrimers as Supports for Organometallic **Catalysts**
AU Naidoo, Kevin J.; Hughes, Samantha J.; Moss, John R.
CS Department of Chemistry, University of Cape Town, Rondebosch, 7701, S. Afr.
SO Macromolecules (1999), 32(2), 331-341 CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English

TI Applications of regularization techniques in electrochemistry
AU Dion, Francois; Lasia, Andrzej
CS Departement de chimie, Universite de Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SO Proceedings - Electrochemical Society (1998), 98-10(Advances in Mathematical Modeling and Simulation of Electrochemical Processes and Oxygen Depolarized Cathodes), 84-94 CODEN: PESODO; ISSN: 0161-6374
PB Electrochemical Society
DT Journal
LA English

TI Electrochemical diffusion: a fast and efficient technique to determine true surface areas in **fractal** surfaces of powder **catalysts**
AU Saffarian, H.; Srinivasan, R.; Gilman, S.; Chu, D.
CS Applied Physics Laboratory, The Johns Hopkins University, Laurel, MD, 20723, USA
SO Proceedings of the Power Sources Conference (1998), 38th, 481-484 CODEN: PPOCFD
PB National Technical Information Service
DT Journal
LA English

TI Influence of structural heterogeneity on selectivity in **fractal catalyst** structures
AU Rigby, Sean P.; Gladden, Lynn F.
CS Department of Chemical Engineering, University of Cambridge, Cambridge, CB2 3RA, UK
SO Journal of Catalysis (1998), 180(1), 44-50 CODEN: JCTLA5; ISSN: 0021-9517

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LA English

TI The influence of the **catalyst** composition on the structure of silica aerogels
AU Bierska, B.; Pajak, L.; Lagiewka, E.
CS Institute of Physics and Chemistry of Metals, University of Silesia, Katowice, 40-007, Pol.
SO Applied Crystallography (1998), 17th, 220-223 CODEN: APCRE2
PB World Scientific Publishing Co. Pte. Ltd.
DT Journal
LA English

TI Development of **fractal** kinetic theory for enzyme- **catalyzed** reactions and implications for the design of biochemical pathways
AU Savageau, Michael A.
CS Department of Microbiology and Immunology, The University of Michigan Medical School, Ann Arbor, MI, 48109-0620, USA
SO BioSystems (1998), 47(1,2), 9-36 CODEN: BSYMBO; ISSN: 0303-2647
PB Elsevier Science Ireland Ltd.
DT Journal
LA English

TI **Fractal** analysis of the shrinking-core model for gas-solid reactions
AU Zhu, Jianjun; Lin, Xiping; Shao, Hui
CS Dep. Chem. Eng., Jiangsu Inst. Petrochem. Technol., Changzhou, 213016, Peop. Rep. China
SO Shiyou Huagong (1998), 27(7), 497-502 CODEN: SHHUE8; ISSN: 1000-8144.
PB Beijing Huagong Yanjiuyuan
DT Journal
LA Chinese

TI The effect of gel precursor structures on the properties of spray dried particles
AU Denny, P. J.; Handley, T. T. J.
CS Department of Chemical Engineering, University of Bradford, West Yorkshire, UK
SO World Congress on Particle Technology 3, Brighton, UK, July 6-9, 1998 (1998), 1994-2004 Publisher: Institution of Chemical Engineers, Rugby, UK. CODEN: 66PSA9
DT Conference; (computer optical disk)
LA English

TI Effect of multifractalities of **catalyst** surface: a Monte Carlo study of **catalytic** CO oxidation

AU Park, H.; Lee, S.

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Review Articles

SO Surface Science (1998), 411(1/2), 1-9 CODEN: SUSCAS; ISSN: 0039-6028

PB Elsevier Science B.V.

DT Journal

LA English

TI A low frequency Raman study of fractons in partially densified silica aerogels

AU Anglaret, Eric; Beurmoies, Isabelle; Duffours, Laurent; Levelut, Claire; Foret, Marie; Delord, Pierre; Woignier, Thierry; Phalippou, Jean; Pelous, Jacques

CS Laboratoire des Verres, Universite Montpellier II, Montpellier, Fr.

SO Journal of Non-Crystalline Solids (1998), 225, 248-253 CODEN: JNCSBJ; ISSN: 0022-3093

PB Elsevier Science B.V.

DT Journal

LA English

TI Sol formation rates in acid **catalyzed** titanium isopropoxide water reaction in isopropanol

AU Wu, Kuan-Ting; Spencer, H. Garth

CS Department of Chemistry, Clemson University, Clemson, SC, 29634-1905, USA

SO Journal of Non-Crystalline Solids (1998), 226(3), 249-255 CODEN: JNCSBJ; ISSN: 0022-3093

PB Elsevier Science B.V.

DT Journal

LA English

TI Correlation of the structural properties of sulfide **catalysts** with their reactivity for methanol synthesis. (II). Characterization of the **catalyst** morphology by the theory of **fractal geometry**

AU Wang, Yanji; Zhang, Jiyan; Chang, Liu

CS Department Chemical Engineering, Hebei University Technology, Tianjin, 300130, Peop. Rep. China

SO Huagong Xuebao (Chinese Edition) (1998), 49(3), 329-334 CODEN: HUKHAI; ISSN: 0438-1157

PB Huaxue Gongye Chubanshe

DT Journal

LA Chinese

TI The validation of **fractal** structural models of porous media by NMR experimental techniques

AU Rigby, Sean P.; Gladden, Lynn F.

CS ICI Katalco, Cleveland, TS23 1LB, UK

SO IChemE Research Event, A Two-Day Symposium, Newcastle upon Tyne, Apr. 7-8, 1998 (1998), 1559-1569 Publisher: Institution of Chemical Engineers, Rugby, UK. CODEN: 65ZTAL

TI A microcatalytic support realized by LIGA technique: the Devil's Comb

AU Basrour, Skandar; Mougin, Pascal; Pons, Michel; Bernede, Philippe; Daniau, William; Villiermaux, Jacques

CS Institut des Microtechniques de Franche-Comte, Besancon, Fr.

SO Transducers 97, International Conference on Solid-State Sensors and Actuators, Chicago, June 16-19, 1997 (1997), Volume 1, 649-652 Publisher: Institute of Electrical and Electronics Engineers, New York, N. Y. CODEN: 66KBAZ

DT Conference

LA English

TI Synergetic effect of carboxylic acid functional groups and fractal surface characteristics for efficient dye sensitization of titanium oxide

AU Falaras, Polycarpos

CS Institute of Physical Chemistry, NCSR "Demokritos", Aghia Paraskevi Attikis, 153 10, Greece

SO Solar Energy Materials and Solar Cells (1998), 53(1-2), 163-175 CODEN: SEMCEQ; ISSN: 0927-0248

PB Elsevier Science B.V.

DT Journal

LA English

TI Theoretical analysis of two kinds of boundary conditions for steady first-order isothermal diffusion reactions in porous solid catalyst particles with fractal geometry symmetry model

AU Shen, Yuenian; Duan, Yiwen; Zou, Ceqian; Hu, Ruisheng; Wu, Di; Chen, Liping; Fan, Haiyan

CS Department of Chemistry, NeiMongol University, Hohhot, 010021, Peop. Rep. China

SO Neimenggu Daxue Xuebao, Ziran Kexueban (1998), 29(2), 181-188 CODEN: NDZKEJ; ISSN: 1000-1638

PB Neimenggu Daxue Xuebao Bianjibu

DT Journal

LA English

TI Fractal kinetics and surface reactions

AU Moiny, F.; Dumont, Martine; Dagonnier, R.

CS Faculte des Sciences, Universite de Mons-Hainaut, B-7000 MONS, Belg.

SO Journal of Chemical Physics (1998), 108(11), 4572-4581 CODEN: JCPSA6; ISSN: 0021-9606

PB American Institute of Physics

DT Journal

LA English

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AU Yang, Lingfa; Hou, Zhonghui; Xin, Houwen
CS Dep. Chem. Phys., Univ. Sci. Technol. China, Hefei, 230026, Peop. Rep. China
SO Huaxue Wuli Xuebao (1998), 11(1), 62-68 CODEN: HWXUE4; ISSN: 1003-7713
PB Zhongguo Kexue Jishu Daxue Chubanshe
DT Journal
LA Chinese

TI A study on the chemical heterogeneity of active surface of solid **catalysts**
AU Anon.
CS USA
SO Journal of Colloid and Interface Science (1997), 196(1), 110-112 CODEN: JCISA5;
ISSN: 0021-9797
PB Academic Press
DT Journal
LA English

TI **Catalytic** behavior of Cu-based **catalysts** with surface **fractal** dimension for high alcohols
AU Li, Chunhu; Zhao, Jiusheng; Wang, Daxiang; Zhu, Chunli; Zhang, Liu
CS Inst. of Chem. Eng. for Coal, Taiyuan University of Technology, Taiyuan, 030024, Peop. Rep. China
SO Taiyuan Gongye Daxue Xuebao (1997), 28(3), 78-82, 86 CODEN: TGDXEZ; ISSN: 1000-1611
PB Taiyuan Gongye Daxue
DT Journal
LA Chinese

TI Deterministic chaos in reaction engineering, II: Application to fluidized bed **catalytic** reactors
AU Abashar, M. E. E.; Narsingh, U.; Judd, M. R.
CS React. Fluidization Eng. Group (RFEG), Dep. Chem. Eng., Univ. Durban-Westville, Durban, X54001, S. Afr.
SO South African Journal of Chemical Engineering (1997), 9(2), 1-20 CODEN: SACEEM; ISSN: 1026-9185
PB South African Institute of Chemical Engineering
DT Journal
LA English

TI The effectiveness of mass **fractal** **catalysts**
AU Coppens, Marc-Olivier; Froment, Gilbert F.
CS Laboratorium voor Petrochemische Techniek, Universiteit Gent, Ghent, B-9000, Belg.
SO Fractals (1997), 5(3), 493-505 CODEN: FRACEG; ISSN: 0218-348X
PB World Scientific Publishing Co. Pte. Ltd.

TI Amorphous porous materials and manufacture of same by sol-gel process.
IN Tamura, Takamitsu; Fujitsu, Masako; Obe, Kazuo; Aikawa, Kyoko; Kaneko, Katsumi
PA Lion Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 16 pp. CODEN: JKXXAF
DT Patent
LA Japanese
JP 09295811

TI Mechanism Discrimination in Heterogeneous **Catalytic** Reactions: **Fractal** Analysis
AU Khorasheh, Farhad; Radmanesh, Ramin; Kazemeini, Mohammad
CS Department of Chemical Engineering, Sharif University of Technology, Tehran, Iran
SO Industrial & Engineering Chemistry Research (1998), 37(2), 362-366 CODEN: IECRED;
ISSN: 0888-5885
PB American Chemical Society
DT Journal
LA English

TI The kinetics of gasification of microporous carbon with oxygen: a **fractal** approach
AU Gordeeva, L. G.; Prokop'ev, S. I.; Okkel', L. G.; Zaikovskii, V. I.; Kolomiichuk, V. N.;
Aristov, Yu. I.
CS Boreskov Inst. Catalysis, Russian Acad. Scis., Novosibirsk, 630090, Russia
SO Kinetics and Catalysis (Translation of Kinetika i Kataliz) (1997), 38(6), 840-847
CODEN: KICAA8; ISSN: 0023-1584
PB MAIK Nauka/Interperiodica Publishing
DT Journal
LA English

TI Determination of the **fractal** dimension of particle surface by chemical kinetic method
AU Guo, Xiangyun; Zhong, Bing; Peng, Shaoyi
CS Inst. Coal Chem., Chinese Acad. Sci., Taiyuan, 030001, Peop. Rep. China
SO Wuli Huaxue Xuebao (1997), 13(1), 52-55 CODEN: WHXUEU; ISSN: 1000-6818
PB Beijing Daxue Chubanshe
DT Journal
LA Chinese

TI A comparison of reaction rates in mass **fractal** and nonfractal **catalysts**
AU Coppens, M.-O.; Froment, G. F.
CS Laboratorium Petrochemische Techniek, Universiteit Gent, Ghent, B-9000, Belg.
SO Fractals and Chaos in Chemical Engineering, Proceedings of the International CFIC 96
Conference, Rome, Sept. 2-5, 1996 (1997), Meeting Date 1996, 15-26. Editor(s): Giona,

Review Articles

DT Conference

LA English

TI Application of **fractal** in **catalyst** selection and **catalytic** activity evaluation

AU Ji, Hongbing; Lin, Weiming

CS Chem. Eng. Dep., South China Univ. Technol., Canton, 510641, Peop. Rep. China

SO Huagong Xuebao (Chinese Edition) (1997), 48(4), 453-456 CODEN: HUKHAI; ISSN: 0438-1157

PB Huaxue Gongye Chubanshe

DT Journal

LA Chinese

TI Surface **fractal** dimension by nitrogen adsorption of microporous sol-gel-processed SiO₂ ceramics

AU Agren, P.; Rosenholm, J. B.

CS Department Physical Chemistry, Abo Akademi University, Turku, SF-20500, Finland

SO Progress in Colloid & Polymer Science (1997), 105(Trends in Colloid and Interface Science XI), 66-71 CODEN: PCPSD7; ISSN: 0340-255X

PB Steinkopff

DT Journal

LA English

TI Homoclinicity in the dynamics of forced fluidized bed **catalytic** reactors

AU Abashar, M. E.; Elnashaie, S. S. E. H.; Hughes, R.

CS Chemical Engineering Department, University of Durban, Durban, 4000, S. Afr.

SO Chaos, Solitons & Fractals (1997), 8(10), 1655-1684 CODEN: CSFOEH; ISSN: 0960-0779

PB Elsevier

DT Journal

LA English

TI Heterogeneous reactions over **fractal** surfaces: a multifractal scaling analysis

AU Lee, Shyi-Long; Lee, Chung-Kung

CS Dep. Chem., National Chung-Cheng Univ., Chiayi, 62117, Taiwan

SO International Journal of Quantum Chemistry (1997), 64(3), 337-350 CODEN: IJQCB2; ISSN: 0020-7608

PB Wiley

DT Journal

LA English

TI **Fractal** kinetic reaction of enzymes

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SO Beijing Daxue Xuebao, Ziran Kexueban (1996), 32(6), 756-759 CODEN: PCTHAP;
ISSN: 0479-8023

PB Beijing Daxue Chubanshe

DT Journal

LA Chinese

TI Reaction rates in **fractal** vs. uniform catalysts with linear and nonlinear kinetics

AU Gavrilov, C.; Sheintuch, M.

CS Dept. Chemical Engineering Technion, Haifa, 32000, Israel

SO AIChE Journal (1997), 43(7), 1691-1699 CODEN: AIChEJ; ISSN: 0001-1541

PB American Institute of Chemical Engineers

DT Journal

LA English

TI Propagation of radiation defects to a fractally rough surface

AU Okunev, A. G.; Aristov, Yu. I.

CS Siberian Division, Boreskov Institute of Catalysis, Russian Academy of Sciences,
Novosibirsk, 630090, Russia

SO High Energy Chemistry (Translation of Khimiya Vysokikh Energii) (1997), 31(4), 229-
232 CODEN: HIECAP; ISSN: 0018-1439

PB MAIK Nauka/Interperiodica

DT Journal

LA English

TI Study on **catalytic** oxidation and reforming of CH₄, CO₂ and O₂ to syngas. I. **Catalyst**
selection

AU Ji, Hongbing; Song, Yibing; Lin, Weiming

CS Dep. Chem. Eng., South China Univ. Sci. and Technol., Canton, 510641, Peop. Rep.
China

SO Tianranqi Huagong (1996), 21(6), 9-11 CODEN: THTKEF; ISSN: 1001-9219

PB Tianranqi Huagong Bianjibu

DT Journal

LA Chinese

TI **Fractal** dimension of platinum particles dispersed in highly porous carbonized
polyacrylonitrile microcellular foam

AU Ye, Siyu; Vijh, Ashok K.; Dao, Le H.

CS IREQ Institut Varennes d'Hydro-Quebec, Varennes, QC, J3X 1S1, Can.

SO Journal of the Electrochemical Society (1997), 144(5), 1734-1738 CODEN: JESOA; ISSN: 0013-4651

PB Electrochemical Society

DT Journal

LA English

TI Monte Carlo simulations of **catalytic** CO oxidation on **fractal** surfaces of dimension between two and three

AU Park, Hwangseo; Kim, Hojing; Lee, Sangyoub

CS Dep. Chem. and Cent. Mol. Cata., Seoul Natl. Univ., Seoul, 151-742, S. Korea

SO Surface Science (1997), 380(2/3), 514-521 CODEN: SUSCAS; ISSN: 0039-6028

PB Elsevier

DT Journal

LA English

TI Multifractals in surface **catalytic** reaction

AU Xin, Libo; Yang, Lingfa; Hou, Zhonghuai; Xin, Houwen

CS Dep. Chem. Phy., China Univ. Sci. Technol., Hefei, 230026, Peop. Rep. China

SO Huaxue Tongbao (1997), (6), 36-38 CODEN: HHTPAU; ISSN: 0441-3776

PB Kexue

DT Journal

LA Chinese

TI Selective electrocatalytic hydrogenation of 2-cyclohexen-1-one to cyclohexanone

AU Dabo, P.; Mahdavi, B.; Menard, H.; Lessard, J.

CS Cent. Rech. Electrochimie Electrocatalyse, Univ. Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.

SO Electrochimica Acta (1997), 42(9), 1457-1459 CODEN: ELCAAV; ISSN: 0013-4686

PB Elsevier

DT Journal

LA English

TI Texture characterization of SiO₂-ZrO₂ aerogels by SAXS, image analysis of TEM and N₂ adsorption-desorption

AU Blacher, S.; Tihon, P.; Pirard, R.; Pirard, J. P.; Diez, B.; Sobry, R.; van den Bosshe, G.; Brouers, F.; Sahouli, B.

CS Genie Chimique, Liege Univ., Liege, B-4000, Belg.

SO Proceedings of SPIE-The International Society for Optical Engineering (1997), 3095(X-Ray Investigations of Polymer Structures), 187-192 CODEN: PSISDG; ISSN: 0277-786X

PB SPIE-The International Society for Optical Engineering

DT Journal

LA English

TI Radiation **catalysis**: defect transport towards a fractally rough surface

AU Okunev, A. G.; Aristov, Yu. I.

CS Federal Scientific Center, Boreskov Inst. Catalysis, Novosibirsk, 630090, Russia

SO Reaction Kinetics and Catalysis Letters (1996), 58(2), 349-357 CODEN: RKCLAU

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DT Journal

LA English

TI Diffusion and reaction in percolating pore networks

AU Andrade, J. S., Jr.; Street, D. A.; Shibusa, Y.; Havlin, S.; Stanley, H. E.

CS Departamento de Fisica, Universidade Federal do Ceara, Fortaleza, 60451-970, Brazil

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1997), 55(1-B), 772-777 CODEN: PLEEE8; ISSN: 1063-651X

PB American Physical Society

DT Journal

LA English

TI Catalytic reactions at an artificial fractal interface: Simulation with the Devil's Comb

AU Mougou, Pascal; Pons, Michel; Villermaux, Jacques

CS Laboratoire des Sciences du Genie Chimique - CNRS, Ecole Nationale Supérieure des Industries Chimiques - INPL, 1, rue Grandville, BP 451, 54 001, Nancy, Fr.

SO Chemical Engineering Journal (Lausanne) (1996), 64(1), 63-68 CODEN: CMEJAJ; ISSN: 0300-9467

PB Elsevier

DT Journal

LA English

TI Catalyst design accounting for the fractal surface morphology

AU Coppens, Marc-Olivier; Froment, Gilbert F.

CS Laboratorium voor Petrochemische Techniek, Universiteit Gent, Krijgslaan 281, B-9000, Ghent, Belg.

SO Chemical Engineering Journal (Lausanne) (1996), 64(1), 69-76 CODEN: CMEJAJ; ISSN: 0300-9467

PB Elsevier

DT Journal

LA English

TI Fractals and patterns in catalysis

AU Sander, L. M.; Ghaisas, S. V.

CS Department of Physics, University of Michigan, Ann Arbor, MI, 48109, USA

SO Physica A: Statistical and Theoretical Physics (Amsterdam) (1996), 233(3-4, Pattern Formation, Fractals and Statistical Mechanics), 629-639 CODEN: PHYADX; ISSN: 0378-4371

PB Elsevier

DT Journal

LA English

Use of fractal geometry or box counting methods to describe catalysts - July 30, 2003

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Review Articles

AU Puncochar, M.; Drahos, J.; Slezak, J.

CS Institute of Chemical Process Fundamentals, Acad. Sci. Czech Rep., 165 02, Prague, 6, Czech.

SO Chemical Engineering Journal (Lausanne) (1996), 64(1), 1-5 CODEN: CMEJAJ; ISSN: 0300-9467

PB Elsevier

DT Journal

LA English

TI **Fractal structure in base-catalyzed silica aerogels examined by TEM, SAXS and porosimetry**

AU Aristov, Yu. I.; Lisitsa, N.; Zaikovski, V. I.; Lorenc, J.; Jarzebski, A. B.

CS Federal Scientific Center, Boreskov Inst. Catalysis, Novosibirsk, 630090, Russia

SO Reaction Kinetics and Catalysis Letters (1996), 58(2), 367-375 CODEN: RKCLAU; ISSN: 0304-4122

PB Akademiai Kiado

DT Journal

LA English

TI **Local reactivity limited aggregation**

AU Hasmy, Anwar; Anglaret, Eric; Jullien, Remi

CS Centre d'Orsay, Universite Paris-Sud, Orsay, 91405, Fr.

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1996), 54(4-B), 4454-4457 CODEN: PLEEE8; ISSN: 1063-651X

PB American Physical Society

DT Journal

LA English

TI **Analysis by size exclusion chromatography (SEC) of catalytic materials: The fractal properties and the pore size distribution of pumice**

AU Duca, Dario; Deganello, Giulio

CS Istituto di Chimica e Tecnologia dei Prodotti Naturali del CNR and Dipartimento di Chimica Inorganica, Universita di Palermo, Via Archirafi 26-28, Palermo, 90123, Italy

SO Journal of Molecular Catalysis A: Chemical (1996), 112(3), 413-421 CODEN: JMCCF2; ISSN: 1381-1169

PB Elsevier

DT Journal

LA English

TI **Disordered Molecular Sieve with Branched Mesoporous Channel Network**

AU Ryoo, Ryong; Kim, J. M.; Ko, C. H.; Shin, C. H.

CS Department of Chemistry, KAIST, Taejon, 305-701, S. Korea

SO Journal of Physical Chemistry (1996), 100(45), 17718-17724 CODEN: JPCHAX; ISSN: 1063-4259

Review Articles

DT Journal

LA English

TI Monte Carlo simulation of the CO + NO reaction

AU Kortlueke, Olaf; von Niessen, Wolfgang

CS Inst. Physikalische Theoretische Chem., Technische Univ. Braunschweig, Braunschweig, D-38106, Germany

SO Journal of Chemical Physics (1996), 105(11), 4764-4774 CODEN: JCPSA6; ISSN: 0021-9606

PB American Institute of Physics

DT Journal

LA English

TI NMR imaging studies of transport heterogeneity and anisotropic diffusion in porous alumina pellets

AU Rigby, S. P.; Cheah, K-Y.; Gladden, L. F.

CS University of Cambridge, Department of Chemical Engineering, Pembroke Street, Cambridge, CB2 3RA, UK

SO Applied Catalysis, A: General (1996), 144(1-2), 377-388 CODEN: ACAGE4; ISSN: 0926-860X

PB Elsevier

DT Journal

LA English

TI **Fractal** reaction model for combustion regeneration of carbon deposited catalyst

AU Yang, Deming; Lin, Xiping

CS Jiangsu Petrochemical Engineering Institute, Changzhou, 213016, Peop. Rep. China

SO Gaoxiao Huaxue Gongcheng Xuebao (1996), 10(2), 172-177 CODEN: GHGXEG; ISSN: 1003-9015

PB Zhejiang Daxue

DT Journal

LA Chinese

TI Surface reaction of a **fractal** bidimensional catalyst. Simulation of the diffusion regime

AU Mougin, P.; Pons, M.; Villermaux, J.

CS LSGC, ENSIC, Nancy, 54001, Fr.

SO Recents Progres en Genie des Procedes (1995), 9(38, Genie des Procedes dans la Chaine des Polymeres et dans la Chaine Catalytique), 117-122 CODEN: RPGPEX; ISSN: 1166-7478

PB Tec & Doc - Lavoisier

DT Journal

LA French

TI **Fractal aspects in the catalytic reforming of naphtha**

AU Coppens, Marc-Olivier; Froment, Gilbert F.

CS Laboratorium Petrochemische Techniek, Univ. Gent, Ghent, B-9000, Belg.

SO Chemical Engineering Science (1996), 51(10), 2283-2292 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI **Reaction and diffusion at an artificial fractal interface: evidence for a new diffusional regime**

AU Mougou, Pascal; Pons, Michel; Villiermaux, Jacques

CS Laboratoire Sciences Genie Chimique, CNRS, Nancy, 54 001, Fr.

SO Chemical Engineering Science (1996), 51(10), 2293-2302 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI **First-order kinetics in fractal catalysts: renormalization analysis of the effectiveness factor**

AU Giona, M.; Schwalm, W. A.; Adrover, A.; Schwalm, M. K.

CS Dep. Ingegneria Chimica, Univ. Roma, Rome, 00184, Italy

SO Chemical Engineering Science (1996), 51(10), 2273-2282 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI **Image analysis and SAXS characterization of mixed aerogels**

AU Blacher, S.; Tihon, Ph.; Pirard, R.; Pirard, J. P.; Brouers, F.; Sahouli, B.; Diez, B.; Sobry, R.; Van den Bosshe, G.

CS Chemical Engineering, Liege University, Liege, B-4000, Belg.

SO Materials Research Society Symposium Proceedings (1996), 407(Disordered Materials and Interfaces), 33-8 CODEN: MRSPDH; ISSN: 0272-9172

PB Materials Research Society

DT Journal

LA English

TI **Investigation of aggregate structures on length scales from about 5 to 10,000 Å**

AU Schmidt, Paul-W.; Ehruburger-Dolle, Françoise; Pfeifer, Peter; Rieker, Thomas

Use of fractal geometry or box counting methods to describe catalysts - July 30, 2003

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Review Articles

SO Materials Research Society Symposium Proceedings (1996), 407(Disordered Materials and Interfaces), 399-404 CODEN: MRSPDH; ISSN: 0272-9172

PB Materials Research Society

DT Journal

LA English

TI Surface characteristics and **catalytic** activity of Al-Pillared (AZA) and Fe-Al-pillared (FAZA) clays for isopropanol decomposition

AU Ladavos, A. K.; Trikalitis, P. N.; Pomonis, P. J.

CS Department of Chemistry, University of Ioannina, 45332, Ioannina, Greece

SO Journal of Molecular Catalysis A: Chemical (1996), 106(3), 241-54 CODEN: JMCCF2; ISSN: 1381-1169

PB Elsevier

DT Journal

LA English

TI Propagation of a wavepacket on a model **fractal** lattice

AU Chattaraj, P. K.; Nath, S.

CS Department of Chemistry, Indian Institute of Technology, Kharagpur, 721 302, India

SO Pramana (1995), 45(6), 545-60 CODEN: PRAMCI; ISSN: 0304-4289

PB Indian Academy of Sciences

DT Journal

LA English

TI **Fractals** and model **catalysts**

AU Bennett, Carroll, O.; Connor, W. Curtis

CS Department of Chemical Engineering, University of Connecticut, Storrs, CT, 06269-3222, USA

SO Journal of Porous Materials (1995), 2(2), 163-70 CODEN: JPMAFX; ISSN: 1380-2224

PB Kluwer

DT Journal

LA English

TI Simulation of complex dynamic behavior during N₂O **catalytic** decomposition

AU Guo, Xiangyun; Zhong, Bing; Peng, Shaoyi

CS Inst. Coal Chem., Chinese Acad. Sci., Taiyuan, 030001, Peop. Rep. China

SO Wuli Huaxue Xuebao (1995), 11(10), 873-5 CODEN: WHXUEU; ISSN: 1000-6818

PB Beijing Daxue Chubanshe

DT Journal

LA Chinese

Review Articles

AU Lee, Chung-Kung; Lee, Shyi-Long

CS Department of Environmental Engineering, Van-Nung Institute of Technology, Chungli, 32054, Taiwan

SO Surface Science (1995), 339(1/2), 171-81 CODEN: SUSCAS; ISSN: 0039-6028

PB Elsevier

DT Journal

LA English

TI **Fractal** analysis of catalyst NiO/ α -Al₂O₃

AU Zhou, Yong-Chao; Wang, Hua-Ming; Yu, Hua-Gen; Cheng, Ji-Yuan

CS Chengdu Institute of Organic Chemistry, Academia Sinica, Chengdu, 610015, Peop. Rep. China

SO Journal of Natural Gas Chemistry (1995), 4(4), 434-8 CODEN: JGCHE8; ISSN: 1003-9953

PB Chengdu Institute of Organic Chemistry, Academia Sinica

DT Journal

LA English

TI Porous texture characteristics of a homologous series of base- **catalyzed** silica aerogels

AU Jarzebski, Andrzej B.; Lorenc, Jaroslaw; Aristov, Yuri I.; Lisitza, Natalia

CS Polish Academy of Sciences, Institute of Chemical Engineering, Gliwice, 44-100, Pol.

SO Journal of Non-Crystalline Solids (1995), 190(3), 198-205 CODEN: JNCSBJ; ISSN: 0022-3093

PB Elsevier

DT Journal

LA English

TI **Catalytic** interface erosion

AU Meng, Hsin-Fei; Cohen, E. G. D.

CS The Rockefeller University, New York, NY, 10021, USA

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1995), 51(4-B), 3417-26 CODEN: PLEEE8; ISSN: 1063-651X

PB American Physical Society

DT Journal

LA English

TI Characterization of structural inhomogeneities in porous media

AU Gladden, Lynn F.; Hollewand, Michael P.; Alexander, Paul

CS Dep. Chemical Eng., Univ. Cambridge, Cambridge, CB2 3RA, UK

SO AIChE Journal (1995), 41(4), 894-906 CODEN: AICEAC; ISSN: 0001-1541

PB American Institute of Chemical Engineers

DT Journal

LA English

TI Investigation of dynamic scaling in a mutually self-similar series of base-catalyzed aerogels

AU Anglaret, E.; Hasmy, A.; Courtens, E.; Pelous, J.; Vacher, R.

CS Lab. Sci. Mater. Vitreux, Univ. Montpellier II, Montpellier, F-34095, Fr.

SO Europhysics Letters (1994), 28(8), 591-6 CODEN: EULEEJ; ISSN: 0295-5075

PB Editions de Physique

DT Journal

LA English

TI Diffusion and reaction in a fractal catalyst pore- II. Diffusion and first-order reaction

AU Coppens, Marc-Olivier; Froment, Gilbert F.

CS Lab. Petrochem. Tech., Univ. Gent, Ghent, B-9000, Belg.

SO Chemical Engineering Science (1995), 50(6), 1027-39 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI Diffusion and reaction in a fractal catalyst pore- I. Geometrical aspects

AU Coppens, Marc-Olivier; Froment, Gilbert F.

CS Lab. Petrochemische Techniek, Univ. Gent, Ghent, B-9000, Belg.

SO Chemical Engineering Science (1995), 50(6), 1013-26 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI Diffusion and reaction in a fractal catalyst pore - III. Application to the simulation of vinyl acetate production from ethylene

AU Coppens, Marc-Olivier; Froment, Gilbert F.

CS Lab. Petrochem. Tech., Univ. Gent, Ghent, B-9000, Belg.

SO Chemical Engineering Science (1994), 49(24A), 4897-907 CODEN: CESCAC; ISSN: 0009-2509

PB Elsevier

DT Journal

LA English

TI Monte Carlo simulation to study surface diffusion and reaction processes on a fractal catalyst

AU Guo, Xiangyun; Zhong, Bing; Peng, Shaoyi

CS Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001; Peop.

Review Articles

PB Elsevier

DT Journal

LA English

TI Oscillations and chaos in the BZ reactions of o-NH₂C₆H₄COOH system. I. Experimental results and nonlinear dynamics analysis

AU Tang, Yuhong; Liu, Quanliang; Hu, Zhaolin; Hou, Yinlan

CS Graduate Sch., Univ. Sci-Tech. of China, Beijing, 100039, Peop. Rep. China

SO Huaxue Wuli Xuebao (1994), 7(4), 372-9 CODEN: HWXUE4; ISSN: 1003-7713

PB Zhongguo Kexue Jishu Daxue Chubanshe

DT Journal

LA Chinese

TI Aggregates of chemically conjugated microgels regarded as a model of gels

AU Koshiro, Yoshitaka; Morone, Nobuhiro; Fukutomi, Takashi

CS Dep. Polymer Sci., Tokyo Inst. Technol., Tokyo, 152, Japan

SO Polymer Gels and Networks (1995), 3(1), 59-70 CODEN: PGNEEI; ISSN: 0966-7822

PB Elsevier

DT Journal

LA English

TI A multifractal approach to heterogeneous reactions over **fractal** surfaces

AU lee, Chung-Kung; Liang, Wen-Hau; Lee, Shyi-Long

CS Department of Chemistry, National Chung-Cheng University, Chiayi, 621, Taiwan

SO Journal of the Chinese Chemical Society (Taipei) (1994), 41(6), 665-72 CODEN: JCCTAC; ISSN: 0009-4536

PB Chinese Chemical Society

DT Journal

LA English

TI Growth and aging phenomena in silica gels

AU Pantos, E.; West, J.B.; Dokter, W.H.; Van Garderen, H.F.; Beelen, T.P.M.; Van Santen, R.A.

CS SERC, Daresbury Laboratory, Warrington/Cheshire, WA4 4AD, UK

SO Journal of Sol-Gel Science and Technology (1994), 2(1/2/3), 273-6 CODEN: JSGTEC; ISSN: 0928-0707

PB Kluwer

DT Journal

LA English

TI Reactant clustering in heterogeneous catalysis with surface diffusion

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Review Articles

CS Tubitak Marmara Research Center, Research Institute for Basic Sciences, Department of Physics, P.O. Box 21, Gebze, 41470, Turk.

SO Surface Science (1994), 320(1/2), 185-90 CODEN: SUSCAS; ISSN: 0039-6028

PB Elsevier

DT Journal

LA English

TI A comparison of nickel boride and Raney nickel electrode activity in the electrocatalytic hydrogenation of phenanthrene

AU Mahdavi, Behzad; Los, Przemyslaw; Lessard, Marie Josee; Lessard, Jean

CS Departement chimie, Universite Sherbrooke, Sherbrooke, QC J1K 2R1, Can.

SO Canadian Journal of Chemistry (1994), 72(11), 2268-77 CODEN: CJCHAG; ISSN: 0008-4042

DT Journal

LA English

TI Multifractal scaling analysis of the selectivity behavior of a multi-step reaction over DLA surfaces

AU Lee, Chung-Kung; Lee, Shyi-Long

CS Department of Chemistry, National Chung-Cheng University, Chia-Yi, 621, Taiwan

SO Chemical Physics Letters (1994), 226(1-2), 88-92 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

TI Nanostructural investigation of silica aerogels

AU Wang, Jue; Shen, Jun; Wu, Weidong; Zhou, Bin

CS Tongji University, Pohl Institute of Solid State Physics, Shanghai, Peop. Rep. China

SO Materials Research Society Symposium Proceedings (1994), 351(Molecularly Designed Ultrafine/Nanostructured Materials), 183-8 CODEN: MRSPDH; ISSN: 0272-9172

DT Journal

LA English

TI Multifractal scaling analysis of autocatalytic and autopoisoning reactions over DLA surfaces

AU Lee, Chung-Kung; Lee, Shyi-Long

CS Department of Chemistry, National Chung-Cheng University, Ming-Hsiung, Chia-Yi, 621, Taiwan

SO Chemical Physics Letters (1994), 228(6), 539-46 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

Review Articles

AU Arvia, A. J.; Salvarezza, R. C.

CS Inst. Investigaciones Fisicoquimicas Teoricas Aplicadas, La Plata, 1900, Argent.

SO Electrochimica Acta (1994), 39(11-12), 1481-94 CODEN: ELCAAV; ISSN: 0013-4686

DT Journal

LA English

TI **Fractal** characteristic of gas diffusion in porous media

AU Zhang, Baoquan; Li, Shaofen; Liao, Hui

CS Dep. Chem. Eng., Tianjin Univ., Tianjin, 300072, Peop. Rep. China

SO Huagong Xuebao (Chinese Edition) (1994), 45(3), 272-8 CODEN: HUKHAI; ISSN: 0438-1157

DT Journal

LA Chinese

TI **Catalysis** on a fractal lattice: a model for poisoning

AU Clement, Eric; Leroux-Hugon, Patrick; Argyrakis, Panos

CS Lab. Acoustique Optique Matiere Condensee, Univ. Pierre Marie Curie, Paris, 75005, Fr.

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1994), 49(6-A), 4857-64 CODEN: PLEEE8; ISSN: 1063-651X

DT Journal

LA English

TI Diffusion and reaction in a Mandelbrot lung

AU Aris, Rutherford

CS Dep. Chem. Eng. Mater. Sci., Univ. Minnesota, Minneapolis, MN, 55455, USA

SO Chaos, Solitons & Fractals (1991), 1(6), 583-93 CODEN: CSFOEH; ISSN: 0960-0779

DT Journal

LA English

TI Simulation of dispersion of solid on carrier surface

AU Guo, Guolin; Huang, Xiangdong; Tang, Youqi

CS Inst. Phys. Chem., Peking Univ., Beijing, Peop. Rep. China

SO Beijing Daxue Xuebao, Ziran Kexueban (1992), 28(5), 566-74 CODEN: PCTHAP; ISSN: 0479-8023

DT Journal

LA English

TI Hydrogen evolution reaction at composite-coated Raney nickel electrodes in aqueous and aqueous-methanolic solutions

AU Cheong, Amoy Kam; Lasia, Andrzej; Lessard, Jean

CS Cent. Rech. Electrochim. Electrocatal., Univ. Sherbrooke, Sherbrooke, QC, J1K 2R1, Canada

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Review Articles

SO Journal of the Electrochemical Society (1993), 140(10), 2721-5 CODEN: JESOA; ISSN: 0013-4651

DT Journal

LA English

TI Chemical wave front in two dimensions

AU Lemarchand, A.; Lesne, A.; Perera, A.; Moreau, M.; Mareschal, M.

CS Lab. Phys. Theor. Liq., Univ. Pierre et Marie Curie, Paris, 75252, Fr.

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1993), 48(2), 1568-71 CODEN: PLEEE8; ISSN: 1063-651X

DT Journal

LA English

TI Are the pore and surface morphologies of real catalysts fractal?

AU Conner, W. Curtis; Bennett, C. O.

CS Dep. Chem. Eng., Univ. Massachusetts, Amherst, MA, 01003, USA

SO Journal of the Chemical Society, Faraday Transactions (1993), 89(22), 4109-14 CODEN: JCFTEV; ISSN: 0956-5000

DT Journal

LA English

TI Gel transformations in silicas: a combined NMR and SAXS study

AU Dokter, Wim H.; van Garderen, Harold F.; Beelen, Theo P. M.; de Haan, Jan W.; van de Ven, Leo J. M.; van Santen, Rutger A.

CS Schuit Inst. Catal., Univ. Technol. Eindhoven, Eindhoven, 5600 MB, Neth.

SO Colloids and Surfaces, A: Physicochemical and Engineering Aspects (1993), 72, 165-71 CODEN: CPEAEH; ISSN: 0927-7757

DT Journal

LA English

TI Irreversible phase transitions in a surface-reaction model with diffusion- and adsorption-limited reactions

AU Albano, Ezequiel V.

CS Fac. Cienc. Exactas, Univ. Nac. La Plata, La Plata, 1900, Argent.

SO Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics (1993), 48(2), 913-18 CODEN: PLEEE8; ISSN: 1063-651X

DT Journal

LA English

TI A Monte Carlo simulation of the carbon monoxide oxidation on probabilistic fractals

AU Castiès, A.; Mai, J.; von Niessen, W.

Review Articles

SO Journal of Chemical Physics (1993), 99(4), 3082-91 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

TI **Catalysis on a fractal lattice: a model for poisoning**

AU Clement, Eric; Leroux-Hugon, Patrick; Argyrakis, Panos

CS Lab. AOMC, Univ. Pierre et Marie Curie, Paris, 75005, Fr.

SO Materials Research Society Symposium Proceedings (1993), 290(Dynamics in Small Confining Systems), 361-4 CODEN: MRSPDH; ISSN: 0272-9172

DT Journal

LA English

TI **Effect of the rapid thermal decomposition of gibbsite on the fractal dimension of product surfaces**

AU Jovanovic, Nadezda N.; Nikolic, Vojin R.; Novakovic, Tatjana; Terlecki-Baricevic, Ana
CS Dep. Catal. Chem. Eng., Inst. Chem., Technol. Metall., Belgrade, YU-11000, Yugoslavia

SO Journal of the Serbian Chemical Society (1993), 58(3-4), 229-35 CODEN: JSCSEN; ISSN: 0352-5139

DT Journal

LA English

TI **A Monte Carlo simulation for the catalytic oxidation of CO on DLA clusters**

AU Mai, J.; Casties, A.; von Niessen, W.

CS Institut fuer Physikalische und Theoretische Chemie, Technische Universitaet Braunschweig, Braunschweig, W-3300, Germany

SO Chemical Physics Letters (1993), 211(2-3), 197-202 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

TI **Comment on "Critical exponents for the irreversible surface reaction $A + B \rightarrow AB$ with B desorption on homogeneous and fractal media"**

AU Zhuo, Jun; Redner, Sidney

CS Cent. Polym. Stud., Boston Univ., Boston, MA, 02215, USA

SO Physical Review Letters (1993), 70(18), 2822 CODEN: PRLTAO; ISSN: 0031-9007

DT Journal

LA English

TI **Characterization for geometric texture and catalytic properties of vanadium-series**

Review Articles

AU Duan, Shiduo; Lin, Qiang; Wang, Jifen; Zhu, Bin

CS Dep. Chem., Tianjin Univ., Tianjin, 300072, Peop. Rep. China

SO Gaodeng Xuexiao Huaxue Xuebao (1992), 13(10), 1299-301 CODEN: KTHPDM; ISSN: 0251-0790

DT Journal

LA Chinese

TI Characterization of the surface texture of **catalysts** for naphthalene oxidation to phthalic anhydride and study of surface texture model

AU Duan, Shiduo; Yang, Kui

CS Dep. Chem., Tianjin Univ., Tianjin, 300072, Peop. Rep. China

SO Gaodeng Xuexiao Huaxue Xuebao (1992), 13(10), 1313-14 CODEN: KTHPDM; ISSN: 0251-0790

DT Journal

LA Chinese

TI Dynamics of roughness and surface reactions at solid electrodes

AU Arvia, A. J.; Salvarezza, R. C.; Vara, J. M.

CS Inst. Invest. Fisicoquim. Teor. Apl., Univ. La Plata, La Plata, 1900, Argent.

SO Electrochimica Acta (1992), 37(12), 2155-67 CODEN: ELCAAV; ISSN: 0013-4686

DT Journal

LA English

TI On the turbidity of silica gels: aggregation in the presence of Coulomb interactions

AU Martin, James E.; Odinek, Judy

CS Sandia Natl. Lab., Albuquerque, NM, 87185, USA

SO Journal of Colloid and Interface Science (1992), 154(2), 461-80 CODEN: JCISA5; ISSN: 0021-9797

DT Journal

LA English

TI Scaling approach to study diffusion and reaction processes on **fractal catalysts**

AU Gutfraind, Ricardo; Sheintuch, Moshe

CS Chem. Eng. Dep., Technion, Haifa, 32000, Israel

SO Chemical Engineering Science (1992), 47(17-18), 4425-33 CODEN: CESCAC; ISSN: 0009-2509

DT Journal

LA English

TI Study of the critical behavior of an irreversible phase transition in the $A + B \rightarrow AB$ reaction with B desorption on a **fractal surface**

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Review Articles

CS Fac. Cienc. Exactas, Univ. Nac. La Plata, La Plata, 1900, Argent.

SO Physical Review A: Atomic, Molecular, and Optical Physics (1992), 46(8), 5020-5

CODEN: PLRAAN; ISSN: 0556-2791

DT Journal

LA English

TI A model for the **catalytic** oxidation of carbon monoxide on **fractal** lattices

AU Mai, J.; Casties, A.; Von Niessen, W.

CS Inst. Phys. Theor. Chem., Tech. Univ. Braunschweig, Braunschweig, W-3300, Germany

SO Chemical Physics Letters (1992), 196(3-4), 358-62 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

TI Anomalous scaling of diffusion and reaction processes on **fractal catalysts**

AU Gutfraind, R.; Sheintuch, M.

CS Israel Inst. Technol., TECHNION, Haifa, 32000, Israel

SO Chemical Engineering Science (1992), 47(9-11), 2787-92 CODEN: CESCAC; ISSN: 0009-2509

DT Journal

LA English

TI **Fractal** dynamics of the **catalytic** carbon monoxide oxidation - application of **fractal** cellular automata models

AU Plath, Peter Joerg

CS Inst. Angew. Phys. Chem., Univ. Bremen, Bremen, 2800/33, Germany

SO NATO ASI Series, Series B: Physics (1991), 258(Large-Scale Mol. Syst.), 545-56

CODEN: NABPDS; ISSN: 0258-1221

DT Journal

LA English

TI Oscillations during carbon monoxide oxidation: a Monte Carlo simulation

AU Mukesh, D.

CS Alchemie Res. Cent., Thane, 400 601, India

SO Journal of Catalysis (1992), 133(1), 153-8 CODEN: JCTLA5; ISSN: 0021-9517

DT Journal

LA English

TI **Fractal** and multifractal analysis of the sensitivity of **catalytic** reactions to **catalyst** structure

AU Gutfraind, Ricardo; Sheintuch, Moshe; Avnir, David

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Review Articles

SO Journal of Chemical Physics (1991), 95(8), 6100-11 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

TI Steady-state diffusion and reactions in **catalytic fractal** porous media

AU Elias-Kohav, Tamar; Sheintuch, Moshe; Avnir, David

CS Dep. Chem. Eng., Technion-Israel Inst. Technol., Haifa, 32000, Israel

SO Chemical Engineering Science (1991), 46(11), 2787-98 CODEN: CESCAC; ISSN: 0009-2509

DT Journal

LA English

TI **Fractal** analysis of surface geometry effects on **catalytic** reactions

AU Seri-Levy, Alon; Avnir, David

CS Fritz Haber Res. Cent. Mol. Dyn., The Hebrew Univ. Jerusalem, Jerusalem, 91904, Israel

SO Surface Science (1991), 248(1-2), 258-70 CODEN: SUSCAS; ISSN: 0039-6028

DT Journal

LA English

TI **Fractal** basin boundaries for the forced autocatalator

AU Liu, Junli; Scott, S. K.

CS Sch. Chem., Univ. Leeds, Leeds, LS2 9JT, UK

SO Journal of Chemical Physics (1991), 94(6), 4416-20 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

TI Selectivity behavior of a multistep reaction on a **catalyst** modeled as a DLA **fractal** surface

AU Tambe, S. S.; Badola, P.; Kulkarni, B. D.

CS Chem. Eng. Div., Natl. Chem. Lab., Pune, 411008, India

SO Chemical Physics Letters (1990), 173(1), 67-9 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

TI **Fractal** kinetics in surface reactions

AU Sente, B.; Dumont, M.; Dagonnier, R.

CS Univ. Etat, Mons, B7000, Belg.

SO Vacuum (1990), 41(1-3), 130-3 CODEN: VACUAV; ISSN: 0042-207X

DT Journal

TI Electron spin echo as a tool for investigation of surface structure of finely dispersed **fractal** solids

AU Kutsovskii, Y. E.; Mariasov, A. G.; Aristov, Y. I.; Parmon, V. N.

CS Inst. Catal., Novosibirsk, 630090, USSR

SO Reaction Kinetics and Catalysis Letters (1990), 42(1), 19-24 CODEN: RKCLAU; ISSN: 0304-4122

DT Journal

LA English

TI Different kinds of **fractal** structures in silica aerogels

AU Woignier, T.; Phalippou, J.; Vacher, R.; Pelous, J.; Courtens, E.

CS Lab. Sci. Mater. Vitreux, Univ. Sci. Tech. Languedoc, Montpellier, F34060, Fr.

SO Journal of Non-Crystalline Solids (1990), 121(1-3), 198-201 CODEN: JNCSBJ; ISSN: 0022-3093

DT Journal

LA English

TI **Fractal** study of tertiary structure of proteins

AU Wang, Cunxin; Shi, Yunyu; Huang, Fuhua

CS Cent. Fundam. Phys., Univ. Sci. Technol. China, Anhui, Peop. Rep. China

SO Physical Review A: Atomic, Molecular, and Optical Physics (1990), 41(12), 7043-8
CODEN: PLRAAN; ISSN: 0556-2791

DT Journal

LA English

TI Towards a **fractal** computer graphic basis for characterization of **catalyst** pore structure by image reconstruction

AU Mann, R.; Wasilewski, M. C.

CS Dep. Chem. Eng., UMIST, Manchester, M60 1QD, UK

SO Chemical Engineering Research and Design (1990), 68(A2), 177-84 CODEN: CERDEE; ISSN: 0263-8762

DT Journal

LA English

TI The effect of aggregation on colloid **catalysts**: a **fractal** model

AU Melrose, J. R.

CS Blackett Lab., Imp. Coll., London, SW7 2BZ, UK

SO Journal of Chemical Physics (1990), 92(7), 4595-9 CODEN: JCPSA6; ISSN: 0021-9606

DT Journal

LA English

TI Optimization of heterogeneous-catalyst structure: simulations and experiments with **fractal** and non-fractal systems

AU Avnir, D.; Citri, O.; Farin, D.; Ottolenghi, M.; Samuel, J.; Seri-Levy, A.

CS Inst. Chem., Hebrew Univ., Jerusalem, 91904, Israel

SO Springer Series in Synergetics (1989), 44(Optimal Struct. Heterog. React. Syst.), 65-81

CODEN: SSSYDF; ISSN: 0172-7389

DT Journal

LA English

TI **Fractal** analysis of carbon monoxide hydrogenation over rhodium catalysts

AU Jackson, S. David

CS Res. Technol. Dep., ICI Chem. and Polym. Ltd., Cleveland, TS23 1LB, UK

SO Reaction Kinetics and Catalysis Letters (1989), 39(2), 223-6 CODEN: RKCLAU; ISSN: 0304-4122

DT Journal

LA English

TI Structure sensitivity scaling laws in heterogeneous **catalysis** on dispersed metals. 2. **Fractal** and non-fractal interpretations of the reaction dimension

AU Farin, Dina; Avnir, David

CS Fritz Haber Res. Cent. Mol. Dyn., Hebrew Univ. Jerusalem, Jerusalem, 91904, Israel

SO Proc. - Int. Congr. Catal., 9th (1988), Volume 3, 998-1005. Editor(s): Phillips, M. J.; Ternan, M. Publisher: Chem. Inst. Can., Ottawa, Ont. CODEN: 56NZA9

DT Conference

LA English

TI On the **fractal** structure of silica aerogels

AU Vacher, R.; Woignier, T.; Phalippou, J.; Pelous, J.; Courtens, E.

CS Lab. Sci. Mater. Vitreux, Univ. Sci. Tech. Languedoc, Montpellier, F-34060, Fr.

SO Journal de Physique, Colloque (1989), (C4, Proc. Int. Symp. Aerogels--ISA 2, 2nd, 1988), C4-127/C4-131 CODEN: JPQCAK; ISSN: 0449-1947

DT Journal

LA English

TI The **fractal** dimension as a characteristic for **catalysts**. 3. Mass transfer and fractality in gas-solid reactions

AU Spindler, Herbert; Kaerger, Joerg

CS VEB Leuna-Werke "Walter Ulbricht", Leuna, DDR-4220, Ger. Dem. Rep.

SO Zeitschrift fuer Physikalische Chemie (Leipzig) (1989), 270(2), 225-36 CODEN: ZPCLAH; ISSN: 0323-4479

DT Journal

TI Anomalous transport in disordered media

AU Bunde, Armin

CS Fak. Phys., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.

SO Solid State Ionics (1988), Volume Date 1987, 28-30(Pt. 1), 34-40 CODEN: SSIOD3;
ISSN: 0167-2738

DT Journal

LA English

TI The fractal dimension as a catalyst size characteristic. 2. Fractal description of the surface and pore volume

AU Spindler, Herbert; Ackermann, Wolf Guenter; Kraft, Manfred

CS VEB Leuna-Werke "Walter Ulbricht", Leuna, DDR-4220, Ger. Dem. Rep.

SO Zeitschrift fuer Physikalische Chemie (Leipzig) (1988), 269(6), 1233-9 CODEN:
ZPCLAH; ISSN: 0323-4479

DT Journal

LA German

TI Fractal structure of base catalyzed and densified silica aerogels

AU Vacher, Rene; Woignier, Thierry; Phalippou, Jean; Pelous, Jacques; Courtens, Eric

CS Lab. Sci. Mater. Vitreux, Univ. Sci. Tech. Languedoc, Montpellier, F-34060, Fr.

SO Journal of Non-Crystalline Solids (1988), 106(1-3), 161-5 CODEN: JNCSBJ; ISSN:
0022-3093

DT Journal

LA English

TI The fractal dimension as a catalyst characteristic. I. Mathematical introduction

AU Ackermann, Wolf Guenter; Spindler, Herbert

CS VEB Leuna-Werke "Walter Ulbricht", Leuna, DDR-4220, Ger. Dem. Rep.

SO Zeitschrift fuer Physikalische Chemie (Leipzig) (1988), 269(5), 1000-10 CODEN:
ZPCLAH; ISSN: 0323-4479

DT Journal

LA German

TI On the applicability of fractals and Monte Carlo methods to heterogeneous catalysis

AU Fichtorn, K. A.; Ziff, R. M.; Gulari, E.

CS Dep. Chem. Eng., Univ. Michigan, Ann Arbor, MI, 48105, USA

SO Studies in Surface Science and Catalysis (1988), Volume Date 1987, 38(Catalysis
1987), 883-94 CODEN: SSCTDM; ISSN: 0167-2991

DT Journal

LA English

TI Structure formation in organosilica gels as a function of the chemical properties

AU Himmel, Bernhard; Gerber, Thomas; Buerger, Herbert

CS Sekt. Phys., Wilhelm-Pieck Univ., Rostock, DDR-2500, Ger. Dem. Rep.

SO Rostocker Physikalische Manuskripte (1987), 11, 86-7 CODEN: RPMADH; ISSN: 0138-3140

DT Journal

LA German

TI Comparative studies of fractal dimensions of carbons obtained via small angle x-ray scattering and electrochemical characterization

AU Le Mehaute, Alain; Crepy, Gilles; Hurd, Alan; Schaefer, Dale; Wilcoxon, Jess; Spooner, Steven

CS Div. Energ., Lab. Marcoussis, Marcoussis, 91460, Fr.

SO Comptes Rendus de l'Academie des Sciences, Serie II: Mecanique, Physique, Chimie, Sciences de la Terre et de l'Univers (1987), 304(10), 491-4 CODEN: CRAMED; ISSN: 0764-4450

DT Journal

LA French

TI Surface fractal dimension of small metallic particles

AU Romeu, D.; Gomez, A.; Perez-Ramirez, J. G.; Silva, R.; Perez, O. L.; Gonzalez, A. E.; Jose-Yacaman, M.

CS Inst. Fis., Univ. Nac. Auton. Mexico, Mexico City, 01000, Mex.

SO Physical Review Letters (1986), 57(20), 2552-5 CODEN: PRLTAO; ISSN: 0031-9007

DT Journal

LA English

TI Surface interaction in the platinum- γ -alumina system. V. Effects of atmosphere and fractal topology on the sintering of platinum

AU Rothschild, Walter G.; Yao, H. C.; Plummer, H. K., Jr.

CS Sci. Lab., Ford Mot. Co., Dearborn, MI, 48121, USA

SO Langmuir (1986), 2(5), 588-93 CODEN: LANGD5; ISSN: 0743-7463

DT Journal

LA English

TI Fractal clustering of reactants on a catalyst surface

AU Ziff, Robert M.; Fichthorn, Kristen

CS Dep. Chem. Eng., Univ. Michigan, Ann Arbor, MI, 48109, USA

SO Physical Review B: Condensed Matter and Materials Physics (1986), 34(3), 2038-40 CODEN: PRBMDO; ISSN: 0163-1829

DT Journal

TI Simulation of the effects of **fractal geometry** on the selectivity of heterogeneous **catalysts**

AU Meakin, Paul

CS Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA

SO Chemical Physics Letters (1986), 123(5), 428-32 CODEN: CHPLBC; ISSN: 0009-2614

DT Journal

LA English

TI The organism as bioreactor. Interpretation of the reduction law of metabolism in terms of heterogeneous **catalysis** and **fractal** structure

AU Sernetz, M.; Gelleri, B.; Hofmann, J.

CS Inst. Biochem. Endokrinol., Justus Liebig-Univ. Giessen, Giessen, D-6300, Fed. Rep. Ger.

SO Journal of Theoretical Biology (1985), 117(2), 209-30 CODEN: JTBIAP; ISSN: 0022-5193

DT Journal

LA English

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